U.S. DEPARTMENT OF COMMERCE
National Technical Information Service

PB-284 338

Systems for Rapid Ranking of Environmental Pollutants Selection of Subjects for Scientific and Technical Assessment Reports

Stanford Research Inst., Menlo Park, Calif

Prepared for

Environmental Protection Agency, Washington, D.C.

Jun 78

United States
Environmental Protection
Agency

Office of Health and Ecological
Effects
Washington DC 20460

EPA-600/5-78-012
June 1978

Research and Development

PB 284 338

EPA

Systems for Rapid Ranking of Environmental Pollutants

Selection of Subjects for Scientific and Technical Assessment Reports

REPRODUCED BY
NATIONAL TECHNICAL
INFORMATION SERVICE
U. S. DEPARTMENT OF COMMERCE
SPRINGFIELD, VA. 22161

RESEARCH REPORTING SERIES

Research reports of the Office of Research and Development, U.S. Environmental Protection Agency, have been grouped into nine series. These nine broad categories were established to facilitate further development and application of environmental technology. Elimination of traditional grouping was consciously planned to foster technology transfer and a maximum interface in related fields. The nine series are:

1. Environmental Health Effects Research
2. Environmental Protection Technology
3. Ecological Research
4. Environmental Monitoring
5. Socioeconomic Environmental Studies
6. Scientific and Technical Assessment Reports (STAR)
7. Interagency Energy-Environment Research and Development
8. "Special" Reports
9. Miscellaneous Reports

This report has been assigned to the SOCIOECONOMIC ENVIRONMENTAL STUDIES series. This series includes research on environmental management, economic analysis, ecological impacts, comprehensive planning and forecasting, and analysis methodologies. Included are tools for determining varying impacts of alternative policies, analyses of environmental planning techniques at the regional, state, and local levels, and approaches to measuring environmental quality perceptions, as well as analysis of ecological and economic impacts of environmental protection measures. Such topics as urban form, industrial mix, growth policies, control, and organizational structure are discussed in terms of optimal environmental performance. These interdisciplinary studies and systems analyses are presented in forms varying from quantitative relational analyses to management and policy-oriented reports.

This document is available to the public through the National Technical Information Service, Springfield, Virginia 22161.

TECHNICAL REPORT DATA
(Please read Instructions on the reverse before completing)

1. REPORT NO. EPA-600/5-012	2.	3. RECIPIENT'S ACCESSION NO. PB284338
4. TITLE AND SUBTITLE SYSTEMS FOR RAPID RANKING OF ENVIRONMENTAL POLLUTANTS Selection of Subjects for Scientific and Technical Assessment Reports		5. REPORT DATE June 1978 issuing date 6. PERFORMING ORGANIZATION CODE
7. AUTHOR(S) Stephen L. Brown, Buford R. Holt, and Kirtland E. McCaleb		8. PERFORMING ORGANIZATION REPORT NO.
9. PERFORMING ORGANIZATION NAME AND ADDRESS Stanford Research Institute 333 Ravenswood Avenue Menlo Park, California 94025		10. PROGRAM ELEMENT NO. 11. CONTRACT/GRANT NO. 68-01-2940 Tasks 015 and 023
12. SPONSORING AGENCY NAME AND ADDRESS Environmental Protection Agency 401 M Street, SW Washington, D.C. 20460		13. TYPE OF REPORT AND PERIOD COVERED Final 14. SPONSORING AGENCY CODE EPA/ORD
15. SUPPLEMENTARY NOTES		

16. ABSTRACT

This document reports the results of the development and testing of a system for rapidly ranking environmental pollutants. One potential use for the system is in choosing the most important candidates for Scientific and Technical Assessment Reports (STAR). Of several possible approaches to ranking environmental agents, a system depending on expert opinion but assisted by an objective subsystem was selected for development. The system defines procedures for collecting, processing, and evaluating data on production and use; environmental transport, transformation, and rate; and human health and welfare and ecological effects. A test of the objective subsystem confirmed the utility of the system. Of ten candidate agents, the three highest ranked were cyanides, carbon disulfide, and beryllium.

17. KEY WORDS AND DOCUMENT ANALYSIS

a. DESCRIPTORS	b. IDENTIFIERS/OPEN ENDED TERMS		c. COSATI Field/Group
Contaminants	STAR	Carbonyl Sulfide	6F 6R 6T
Assessments	Priorities	Cyanides	7B 7C 7D
Criteria	Environmental Agents	Heat	12B 18G
Ranking	Hazards	Plutonium	
Systems Analysis	Antimony	Beryllium	
Ecology	Molybdenum	Lithium	
	Cobalt	Carbon Disulfide	

18. DISTRIBUTION STATEMENT Document is available to the public through the National Technical Information Service, Springfield, Virginia 22151	19. SECURITY CLASS *(This Report)* Unclassified	21. NO. OF PAGES 281
	20. SECURITY CLASS *(This page)* Unclassified	22. PRICE PC A13 MF A01

EPA Form 2220-1 (9-73)

U.S. GOVERNMENT PRINTING OFFICE: 1978—260-880/73

June, 1978

EPA-600/5-78-013

SYSTEMS FOR RAPID RANKING
OF ENVIRONMENTAL POLLUTANTS

EPA Contract No. 68-01-2940, Tasks 015, 023

Technical Monitor
Alan P. Carlin

Office of Health and Ecological Effects
Office of Research and Development
U.S. Environmental Protection Agency
Washington, D.C. 20460

DISCLAIMER

This report has been reviewed by the Office of Health and Ecological Effects, and approved for publication. Approval does not signify that the contents necessarily reflect the views and policies of the Environmental Protection Agency, nor does mention of trade names or commercial products constitute endorsement or recommendation for use. This report is available for purchase from the National Technical Information Service, P.O. Box 1553, Springfield, Virginia 22161. The order number is PB258168.

PREFACE

This report was prepared by an interdisciplinary team under the general guidance of Alan P. Carlin, the EPA technical monitor. The SRI team consisted of Howard C. Bailey, David C. Bomberger, Stephen L. Brown (project leader), Kristin M. Clark, Anthony V. Colucci (consultant), Jerie L. Etherton, Peter C. Hall, Buford R. Holt, David H. Liu, William R. Mabey, Kirtland E. McCaleb, David R. Myers, Thomas O. Peyton, Dennis E. Schendel, Lyle M. Schump, Robert V. Steele, Steven H. Traver, and Rose M. Wright.

WARNING: THE DATA REPORTED IN THIS DOCUMENT WITH RESPECT TO VARIOUS POTENTIALLY HAZARDOUS ENVIRONMENTAL AGENTS SHOULD BE USED ELSEWHERE ONLY WITH THE UTMOST CAUTION. THESE DATA WERE GATHERED AS INPUT TO A PRIORITY-SETTING PROCESS AND ARE THUS INCOMPLETE AND LARGELY UNVERIFIED.

CONTENTS

PREFACE iii

LIST OF ILLUSTRATIONS ix

LIST OF TABLES. ix

PART ONE--OVERVIEW. 1

I INTRODUCTION. 3
  - A. Background 3
  - B. Objectives 6
  - C. Method of Approach 6

II SUMMARY 11

III CONCLUSIONS 15

IV RECOMMENDATIONS 19

PART TWO--SYSTEMS FOR RANKING ENVIRONMENTAL POLLUTANTS. 21

V SELECTION OF SYSTEMS FOR DEVELOPMENT. 23
  - A. Ranking Systems. 23
  - B. Assumptions and Criteria 25
  - C. Systems Considered 27
  - D. Expert-Based System. 27
  - E. Screening-Indexing System. 30
  - F. Model-Based System 34
  - G. Selection Rationale. 35

VI A PRIORITY RANKING SYSTEM BASED ON THE USE OF EXPERT GROUPS 37

Preceding page blank

A. Outline of the System. 37
B. Relevant Information and Literature Sources. . . . 38
C. Format for Presenting Data 38
D. Composition of the Expert Committee and Criteria for Their Selection 39
E. Operating Procedures 39
F. Scientific Review Group Operations 40
G. Estimated Operating Costs. 41

VII DEVELOPMENT OF OBJECTIVE SUBSYSTEM. 43
A. Selection of Parameters. 43
B. Basic System Concepts. 44
C. Development of Procedures. 45
D. Operating Personnel and Costs. 46

PART THREE--TEST OF OBJECTIVE SUBSYSTEM. 51

VIII DESCRIPTION OF THE TEST 53
A. Definition of the Agents 53
B. Assignment of Tasks. 54
C. Information Sources. 56
D. Summary of the Findings. 57
E. Sensitivity Analyses 66

IX EVALUATION OF THE TEST. 71
A. Criteria for Evaluation. 71
B. Successes and Failures of the System 71
C. Suggested Improvements 75

APPENDICES

A DATA ELEMENTS FOR THE EXPERT SYSTEM 79

B RECOMMENDED FORMAT FOR PRESENTING DATA TO THE EXPERT COMMITTEE. 85

C RECOMMENDED CRITERIA FOR SELECTING MEMBERS OF THE EXPERT COMMITTEE. 101

D RECOMMENDED EVALUATION SHEET AND PROPOSED METHOD OF USE BY MEMBERS OF THE EXPERT COMMITTEE 107

E PARAMETERS FOR USE IN THE OBJECTIVE SUBSYSTEM 113

F PROCEDURES FOR OBJECTIVE RANKING. 135

G SAMPLE RANKING RESULTS FOR CARBON DISULFIDE AND CYANIDES. 229

H ABBREVIATIONS 279

I REFERENCES. 285

LIST OF ILLUSTRATIONS

1 Overall Structure of the Objective Subsystem 47

F-1 Generalized System Flow Component. 139

LIST OF TABLES

I-1 Published and Planned STAR Documents. 4

I-2 Typical STAR Outline. 5

VI-1 Expert-Based System Costs 42

VII-1 Personnel for Objective Subsystem 48

VII-2 Objective Subsystem Costs 49

VIII-1 Nominated Agents for the Test 53

VIII-2 Representative Compounds Used 55

VIII-3 General Information Compendia 58

VIII-4 Basic Documents 59

VIII-5 Agent Ranks and Reasons 61

VIII-6 Valuation Range 67

VIII-7 Matrix of Value Systems 68

VIII-8 Range of Rankings 68

E-1 Processes and Uses Leading to Release of Pollutants . . . to the Environment. 116

E-2 Data Sources and Units for Release Routes A-N 117

E-3 Release Routes, Data Sources, and Units 119

E-4 Time/Cost Estimates 120

Preceding page blank

Part One

OVERVIEW

I INTRODUCTION

A. Background

The Office of Research and Development (ORD) of the Environmental Protection Agency (EPA) is in the early stages of producing a series of Scientific and Technical Assessment Reports (STARs), each of which will summarize the state of knowledge about an environmental pollutant. These reports, which have extended the concepts embodied in earlier criteria documents for air pollutants and in National Academy of Sciences monographs on specific pollutants, will be used as input to the regulatory process.

The distinguishing characteristic of the STARs is that they assess all information relevant to the EPA regulatory mission, about the behavior of the pollutant in all media and with respect to all targets. A list of published and planned STARs is shown in Table I-1. In examining this list, first it should be remembered that many of the early documents had a different format from that currently in force, and second that the list is very dynamic; consequently, the picture presented in Table I-1 is a snapshot as of early 1976.

An outline for a typical STAR is shown in Table I-2. As this outline indicates, a key feature of the STAR is to provide information that will enable a decision maker to determine the benefits of a contemplated EPA action with respect to the pollutant. This implies that if a STAR is to make much impact the state of knowledge about the pollutant must be relatively good and the selection of candidates for STARs must be made with this fact in mind.

Preceding page blank

Table I-1

PUBLISHED AND PLANNED STAR DOCUMENTS[*]

	EPA Report No.
Issued	
Particulate polycyclic organic matter	600/6-75-001
Manganese	600/6-75-002
Cadmium	600/6-75-003
Vinyl chloride	600/6-75-004
Planned[†]	
Arsenic	
Halomethanes	
Nickel	
Vanadium	

---

[*] As of early 1976.

[†] Partial list.

Having limited resources, EPA can produce only a few STARs each year. This constraint makes it exceedingly important to select as candidates for STARs only those pollutants whose control by EPA would result in the most significant benefits for the nation's environment.

If it is assumed that the selection is based solely on objective (non-political) considerations, which may not always be the case, the best order for STAR production would be to attack first the pollutant with the highest potential for environmental harm avoidable through EPA actions. Under this assumption, the ordering of STAR candidates would correspond to a priority ranking of environmental pollutants needing EPA regulatory attention.

Table I-2

TYPICAL STAR OUTLINE

1. Summary and Conclusions
2. Pollutant Characterization
    - 2.1 Chemical and Physical Properties
    - 2.2 Measurement Techniques
3. Environmental Occurrence and Transport
    - 3.1 Concentrations
    - 3.2 Transformation and Transport Mechanisms
4. Environmental Exposure and Undesirable Effects
    - 4.1 Mechanisms of Exposure
    - 4.2 Mechanisms of Response
    - 4.3 Undesirable Effects
    - 4.4 Environmental Exposure
5. Sources and Controllability
    - 5.1 Sources
    - 5.2 Control Technology and Controllability
    - 5.3 Undesirable Intermedia Effects of Principal Control Measures
6. Overview, Benefits, and Institutional Problems of Control
    - 6.1 Economic Benefits from Control
    - 6.2 Societal/Institutional Constraints on Control
    - 6.3 Overview

The process of ordering the candidates for STARs is far from simple and requires considerable amounts of information about the candidates that will later appear in the STARs themselves. This process consists, at a miminum, of the following steps:

- Nomination of candidate agents.
- Analysis of the importance of STARs for these agents.
- Selection of agents from the candidates.

At this point we have introduced the term agent as being somewhat broader than pollutant. In the remainder of this report, we will use agent to include chemical pollutants, thermal waste, radiation, noise, and other entities affecting the environment.

The nomination step can be either passive, allowing any interested party to nominate candidates, or active, soliciting nominations from experts and searching for agents of general concern.

The analysis should provide guidance to the decision makers in ordering the STARs. Accordingly, it is the systematic portion of the larger process.

The selection step is ultimately the responsibility of the EPA decision makers who will use the STARs. They must use all the information available to them, explicit and implicit, to decide upon the best order.

B. Objectives

The objectives of the study reported in this document were to examine alternative systems for the ordering or priority ranking of agents for STARs, to recommend a preferred system to develop this system for possible implementation by EPA, to test a portion of the system developed on a selected set of agents, and to correct system deficiencies identified in the test. Thus, in effect, the overall objective was the development of a system for rapidly ranking environmental pollutants.

C. Method of Study

In pursuit of these objectives, SRI assembled an interdisciplinary team of scientists and analysts, including two chemical economists, a chemical engineer, two physical chemists, two environmental health scientists, an ecologist, two toxicologists, a mathematician, two literature specialists, and an environmental systems analyst.

The team met with the EPA technical monitor to confirm the direction of the study, and then conducted a survey of various systems for ranking hazards. Three study groups were formed to investigate three different possible systems for the STAR ranking problem; each group included personnel familiar with releases of agents to the environment, fate of agents in the environments, and effects on receptors.

The three systems, based respectively on the judgment of experts, information screening and ordering, and mathematical models, were developed and presented to EPA/ORD in outline format highlighting their advantages and disadvantages. EPA and SRI then selected a hybrid system for further development. This hybrid system is largely dependent upon the systematized judgment of experts who are supported and balanced by a more objective subsystem based on screening and modeling. This hybrid system was then further developed by two study groups, one concentrating on the expert system and the other on the objective subsystem.

After a careful review of the resulting recommended procedures EPA/ORD determined that a test of the recommended system would both measure its utility and identify desirable modifications. At that time, ORD was attempting to recommend candidates for STARs, and a rapid ranking was seen as useful. Because establishment of the expert committees necessary for the full development of the system would be time consuming, it was decided to test only the objective subsystem on the following ten agents:

Antimony

Beryllium

Carbon disulfide[*]

Carbonyl sulfide[*]

Cobalt

Cyanides

Heat from manmade sources

Lithium

Molybdenum

Plutonium

For those agents that included more than one specific chemical compound of concern, the test of the subsystem included at least two compounds believed to be of the most concern.

The method of approach for the test was dictated largely by the nature of the objective subsystem. That is, once the candidates were nominated, the procedures outlined in the subsystem were followed as faithfully as possible, from definition of the agent to ultimate computation of an environmental hazard index and agent ranking. During this operation, records were kept of the steps of the procedure that were undertaken, and notes were taken on difficulties encountered and solutions achieved.

The principal activities of the test were as follows:

- Data Collection. Basic documents on each of the agents were collected as available. These included abbreviated summaries from data compilations (for example, The Toxic Substances List), draft criteria documents (for example, WHO preliminary review on molybdenum), EPA publications (for example, Plutonium: Statement of the Problem), and other readily available documents. Only limited use was made of bibliographic search techniques (for example, some TOXLINE searches were made).

---

[*] These two candidates were of special concern for current standard-setting activities. A separate, more comprehensive, report was prepared on these entitled, "Carbon Disulfide, Carbonyl Sulfide: Literature Review and Environmental Assessment" (Stanford Research Institute, July 1975) (Draft).

- Subsystem Operation. The objective subsystem was followed step-by-step as closely as possible. Where difficulties arose, they were solved on an ad hoc basis.
- Sensitivity Analysis. The principal organized sensitivity analysis was of variations in the assignment of relative values to the effects of the agents. Also, certain steps were repeated by different operators to test the degree of subjectivity inherent; in addition, the entire ranking was reviewed during the report preparation phase, and numerous minor and several major changes were made.
- Appraisal of Test. The results of the test and the methods of achieving them were reviewed by the project team to determine areas of difficulty, recommendations for improvement, successes and failures, and so on.

II SUMMARY

This report concerns the development and testing of a systematic procedure (system) for priority ranking environmental agents as candidates for Scientific and Technical Assessment Reports (STARs) and thus for priority ranking environmental pollutants needing EPA regulatory attention. The development of this system is part of a larger process that will include the nomination of candidate agents, and the final selection by EPA decision makers of agents for STARs.

In the first phase, a number of systematic procedures previously developed for related ranking purposes were surveyed. Selected elements were incorporated into three different system outlines. A system based on expert judgment was seen as being technically and economically feasible as well as acceptable to EPA decision makers, if the expertise represented were sufficiently high. An information screening system with ranking on a combination of several indexes was seen as simple and economical. A system based on a mathematical model was seen as being more objective, explicit, and reproducible. A combination of the expert system and a more objective screening/model subsystem was selected as having the highest potential for further development.

In the second phase, the expert system was developed to provide for the selection of an Expert Committee by EPA with support from a contractor; the compilation of data by the contractor for presentation to the experts; the priority ranking of agents in four categories, by the experts; the summarization of the results by the contractor for consideration by a Scientific Review Group composed of independent, recognized members of the scientific community; and final ranking by the Scientific Review

Preceding page blank

Group. It was estimated that the system could be operated for about \$3,500 per agent or \$120-130,000 annually for about 36 candidate agents.

The objective subsystem is designed to support and calibrate the expert system, and consists of an explicit procedure that tests the state of information about an agent and processes available information on the basis of the outcome of the tests. The information base for the objective subsystem is a subset of the information for the expert system, with a few exceptions. The subsystem has several important subjective elements, including the choice of processes to represent in the model, the values to assign to the predicted effects of the agent, and the option to use ad hoc studies. It was estimated that the subsystem would cost \$50-60,000 per year to operate, in addition to the cost of the expert system.

In the third phase, the objective subsystem was tested on a sample of 10 agents to determine the weaknesses of the system and to confirm or deny the operating cost estimates. Specific agents representative of the generalized agents on the list of candidates were identified. Antimony was represented by antimony trioxide, beryllium by beryllium metal and beryllium oxide, cobalt by cobaltous chloride and cobaltous naphthenate, cyanides by hydrogen, sodium, and potassium cyanides, lithium by lithium carbonate and lithium chloride, molybdenum by molybdenum oxide and molybdenum sulfide, and plutonium by plutonium^{239} (oxide). Carbon disulfide, carbonyl sulfide, and heat were single agents.

Information sources for the priority ranking procedure included both general information compendia covering such aspects as agent properties or toxicology, and basic documents on individual agents, such as criteria documents or EPA reports.

The ranking was successfully completed, at a cost of about \$1,500 per agent, with the following results:

Rank	Agent	Principal Effect
1	Cyanides	Accidental acute toxicity in man
2	Carbon disulfide	Odor (aesthetic annoyance)
3	Beryllium	Lung cancer in man
4	Lithium	Central nervous system disturbance
5	Plutonium	Life-shortening in man
6	Antimony	Heart disease in man
7	Heat	Fish mortality
8	Carbonyl sulfide	Heart disease in man
9	Cobalt	Toxicity in fish
10	Molybdenum	Molybdenosis in cattle

An alternative ranking, that eliminated a critical assumption on the distribution of higher-than-threshold doses, resulted in the following ranked order: carbon disulfide, beryllium, plutonium and cyanides (tied), and heat; all other agents tied with no effects.

A sensitivity analysis showed that the subsystem was not markedly sensitive to assumptions about the relative values of various effects. It was also fairly insensitive to other subjective inputs, such as the choices of sources of release, with the exceptions of the assumption concerning high dose distribution and the choice of what effects should be considered. As an example of the system's sensitivity to effects, if odor problems with carbon disulfide had not been considered, it would have been ranked in seventh position.

The principal difficulties encountered in the test were in the collection and use of information, and a few procedural difficulties. Data were scanty on release factors to the environment, persistence and intermedia transfer, transport and diffusion, and populations at risk. Interpretation of toxicological information was also difficult. An initial problem was overcoming operator unfamiliarity with the system. This problem extended into difficulties in dealing with necessary subjective judgments not forced by the system. Potential improvements to the system were identified as a result of the test, some of which have already been incorporated in the system and are discussed in this report.

It was concluded, in general, that the subsystem is workable and useful, and can be operated with modest resources. Its principal use is in making assumptions and relationships explicit, identifying factors limiting environmental hazards, and spotlighting areas of critical uncertainty. However, the system would benefit from longer lead times and more access to agent nominators. The reliance on subjective inputs is greater than desirable, and the reproducibility and credibility of the system are consequently degraded.

It is recommended that the subsystem be used only as an input to a more comprehensive process such as the expert process described above. If the system is used in this way, it should be improved modestly but continuously. At least 3 months lead time is recommended, and operation under the supervision of a competent and confident environmental generalist is suggested.

III CONCLUSIONS

In the first phase of this study we reached the conclusion that it would be technically and economically feasible to operate a STAR ranking system based on the use of an Expert Committee, and that the output of such a system would be readily acceptable to decision makers if the degree of expertise were sufficiently high. However, we also concluded that the expert system would be much more effective if supported by a more objective subsystem that processed some of the information for presentation to the experts, and further served as a calibration for the judgments of the experts.

In the second phase, we concluded that the expert system should consist of the following major elements:

- EPA, with contractor support, would select an Expert Committee on the basis of specified criteria.
- A contractor would make a systematic compilation of data on about 10 candidates at a time, for submission to the Expert Committee.
- The experts would assign priority ratings in three subject categories and a fourth overall category.
- A contractor would summarize results for submission to an independent Scientific Review Group.
- The Scientific Review Group would decide on a final ranking. The cost of ranking about 36 candidate agents per year was estimated at $120-130,000.

The objective subsystem should be operated in parallel by the EPA contractor and should use a subset of the data collected for the expert system. (Selective augmentation of data in critical areas may be necessary.) The subsystem contains explicit instructions for obtaining and processing data, as well as decisions on the depth of the analysis needed. (The latter depends on the results of the state of information tests.) However, the objective subsystem also contains important subjective elements, which include the processes chosen to be modeled, the values assigned to various predicted effects of the agent, and the necessity for ad hoc studies when critical information is not easily available. We estimate that the subsystem could be operated for about $1,600 per agent or $50-60,000 per year. The overall system could thus be operated for about $170-190,000 per year.

In the third (test) phase, we concluded that the subsystem is workable and useful, with important caveats. No unresolvable difficulty was encountered in the system operation, and the desired ranking was accomplished. The chief use of the subsystem is in making explicit the assumptions and information about environmental hazard potential and thus identifying the limiting factors and areas of uncertainty.

First among the caveats is the observation that the subsystem would benefit from longer lead times, more direct contact with agent nominators, and operator familiarity. The principal ranking effort was accomplished in about 6 weeks, which prevented us from obtaining as many basic documents on the agents as we would have liked. Direct contact with the nominators would have not only enhanced this information gathering process, but would have directed us more accurately to the principal concerns. A moderate amount of effort was expended in making the operators familiar with the system.

Second, and in many ways more important, is the fact that many pieces of information desired for system operation are unavailable, fragmentary, or difficult to interpret. The major areas in which these deficiencies were limiting were:

- Release factors to the environment
- Persistence and intermedia transfer

- Transport and diffusion
- Populations at risk
- Toxicology interpretation.

This situation required more reliance on default values and ad hoc procedures than was anticipated.

Third, the reproducibility of the system, in terms of the necessity for subjective inputs by the operator, is lower than had been hoped. Consequently, the subsystem is probably of low credibility if examined closely. However, if alternative methods of priority ranking were similarly examined, the subsystem would compare favorably. Moreover, it was not found particularly sensitive to variations in the relative valuation of effects or other uncertainties in the inputs.

Finally, as suggested by the subjectivity observed, the success of the subsystem undoubtedly depends markedly on the creativity and boldness of the operators.

IV RECOMMENDATIONS

On the basis of the development and testing of the rapid ranking system for environmental pollutants, we recommend, with qualifications, that EPA/ORD implement the expert system along with the objective subsystem for ranking STAR candidates and for other priority-setting purposes.

Foremost among the qualifications is that the complete expert system has not been tested; therefore, any implementation should be accompanied by an evaluation and an option for termination after a year's operation. Provision for modifying the expert system procedures in response to the evaluation should also be made.

The objective subsystem should be operated only with careful examination of the assumptions and procedures associated with each agent's ranking. If the objective subsystem is used in conjunction with the expert process as recommended, this examination should be automatic.

If the subsystem is to be used at all, it should undergo modest and continuous improvements, spanning at least the first group of improvements listed in Section IX C.

We further recommend that a candidate agent be introduced into the system at least 3 months prior to a required decision on its priority for a STAR, to allow collection of background documents and thoughtful assessment of the data. The ranking should be conducted under the supervision of a confident and competent environmental generalist.

Preceding page blank

Part Two

SYSTEMS FOR RANKING ENVIRONMENTAL POLLUTANTS

Preceding page blank

V SELECTION OF SYSTEMS FOR DEVELOPMENT

The first phase of research leading to this report consisted of an examination of a variety of ranking systems that had purposes similar to the priority ranking of agents for STARs; the development in outline format of three representative systems, showing the advantages and disadvantages of each to be presented to EPA/ORD; and the selection of a hybrid system for further development.

A. Ranking Systems

The purpose of any ranking system related to an action program is to enable decision makers to do the most important things first. In the case of the STARs, EPA desires to summarize first the scientific and technical information on those environmental pollutants (agents) that have the highest potential for harm, so that EPA's regulatory response can achieve the greatest gains as early as possible.

The STAR priority ranking process is composed of three major steps:

- Nomination of candidate agents
- Systematic ranking of candidates
- Selection, using both the systematic ranking and factors beyond its scope, of the agents for which STARs will be prepared.

This report is concerned principally with the second of these steps. However, the importance of the third step is emphasized by the following caveats about systematic ranking procedures. First, systematic approaches tend to be mistrusted because they sometimes give results that are not intuitively evident to the decision maker, and because these results are sometimes wrong. Second, if completely accurate information were available on all agents to be ranked, the need for a systematic approach would be minimal. Hence it is axiomatic that the need to rank implies considerable uncertainty about the information used in the system. Third, this uncertainty implies that the resulting ranking will be imperfect, with some agents of little actual importance high on the list, and conversely, with some important agents low on the list. Finally, every systematic approach has some unavoidable subjective inputs, whether explicit or implicit, and the system can be attacked on these subjective components.

Once a ranking system is accepted as a part of the overall process, however, some fundamental ranking concepts become important. Basically, the output of a ranking system is a list ranked according to some priority. To use such a list, however, one must make selections from it, for example, one might take the first M item from a list of N. Obviously, if one takes M=N (the whole list), it doesn't matter how the list is ordered. In general, as the ratio of M to N decreases, it becomes more and more important to the selection process to have the list ordered correctly.

Ranking can be accomplished ordinally or by an index. In ordinal ranking, paired comparisons are made: Is this item more or less important than this other item? The resulting list is ordered correctly, but no feeling for the relative spacing between adjoining items is generated. This problem is solved by indexed ranking, in which each item (agent) is assigned a quantitative index, and the ranking is achieved by sorting on this index. With such a system, one can see whether item three is twice as important as item one or only 10% more important. All of the systems considered here are based on indexes, although the ways in which they are derived differ considerably.

If the system is to achieve the purposes for which it was designed, the index must correspond well to the actual importance of the agents to the decision maker. That is, the index must represent a unifying value system. For STARs, we attempted to devise a value system in which the important variable was the degree to which EPA actions could improve human health and welfare through control of agents in the environment. Suggestions as to how this might be defined were taken from two National Academy of Sciences (NAS) reports[*][†] as well as from previous studies by Battelle,[‡] SURC,[§] and SRI.[**]

Two very important components of a ranking system must also be recognized. First, the system must specify the methods and sources for obtaining information, and second, it must define the methods for processing and using this information. Both components must be present for success; all too many systems have failed by concentrating on processing methods and ignoring the specification of sources.

B. Assumptions and Criteria

In developing the outlines for the three candidate systems and in choosing among them, we made several assumptions about STARs and the criteria on which the choice should be made.

---

[*] "Principles for Evaluating Chemicals in the Environment," National Academy of Sciences, (1975). (NAS 1975b)

[†] "Assessing Potential Ocean Pollutants," National Academy of Sciences, (1975). (NAS 1975a)

[‡] "Identification Systems for Selecting Chemical Classes as Candidates for Evaluation," EPA-560/1-74-001, Battelle Memorial Institute, (November 1974). (BMI 1974)

[§] "Establishing Environmental Priorities for Synthetic Organic Chemicals: Focusing on the Next PCB's," Paper presented by P. H. Howard, Syracuse University Research Corporation at Seminar on Early Warning Systems for Toxic Substances, (February 1974). (Howard 1974)

[**] "Research Program on Hazard Priority Ranking of Manufactured Chemicals," Stanford Research Institute (April 1975). (SRI 1975)

Some of the following assumptions may seem trivial; however, they are important to our design:

- STARs will be written and used for regulatory purposes. The order in which STARs should be written should be a direct reflection of the importance of the potential regulatory actions that could be taken.
- Importance is defined in terms of beneficial effects on human health and welfare and ecology as determined by environmental quality.
- The feasibility of control will be addressed partly in the final selection process and partly in the STAR preparation process.
- Certain actions require a high state of knowledge about the agent.
- These state-of-knowledge issues will be resolved outside the systematic part of the priority ranking process.
- The universe of agents nominated for ranking will be small but growing. We assume no more than 36 nominations per year.
- The annual rate of STAR production will be between 6 and 24.

In consultation with the EPA technical monitor, we agreed that the following criteria were valuable in selecting among the proposed systems:

- Technical feasibility
- Economic feasibility
- Acceptability to decision makers
- Robustness with respect to uncertain information
- Simplicity and understandability.

The following criteria are somewhat less important than those above:

- Credibility to various interest groups
- Relative objectivity
- Relative explicitness
- Reproducibility and traceability.

C. Systems Considered

Four conceptual types of systems were considered as possibilities for the STAR ranking.

An expert-based system would use the knowledge of recognized experts to choose among the nominated agents. Although the expert opinion might be based on objective information, the processing of that information would be largely subjective and implicit.

A screening-based system would consist of a series of questions to be answered about the agent. Depending on the answers to the questions, the candidate agents would be sorted into various groups, and the groups ranked by subjective means. The sorting would be done on the basis of objective data.

An index-based system would assign several indices to the agent, each based on objective information about the agent. These individual indices would be combined by subjective rules and weighting factors.

A model-based system would attempt to construct a mathematical model of the processes that cause an agent to be hazardous to human health and welfare and/or to ecosystems. The subjective elements of a model-based system would include the processes to be emphasized and the values to be placed on various predicted effects.

It was found that no pure system satisfied the selection criteria very well. Several hybrids were examined, and the final three candidates emphasized experts, screening-indexing, and models, respectively.

D. Expert-Based System

The expert-based priority ranking system was based on an Expert Committee, an EPA contractor charged with providing input to the Expert Committee and systematizing its output for presentation, and a Scientific

Review Group, such as a suitable National Academy of Sciences committee, which would do the actual priority ranking.

Under this system the EPA contractor would start by gathering available relevant information from a selected group of sources on the chemicals* of interest and putting this information in standarized form for consideration by a committee of experts selected on the basis of a pre-established set of criteria. Each expert would be asked to give his individual estimate of the severity of the potential environmental problems associated with each chemical. These estimates would be done on a numerical scale (accompanied by explanatory supporting text) for certain categories of information and on an overall basis for the chemical. They would be combined by an EPA contractor into a composite estimate and accompanying text for submission to the Scientific Review Group which would be asked to review the estimates and to make recommendations concerning the priority of each chemical in the preparation of STAR documents.

The data to be gathered should include information such as that included in the UN-sponsored International Register of Potentially Toxic Chemicals (IRPTC), the European Economic Committees-sponsored Environmental Chemical Data and Information Network (ECDIN), and the United Kingdom Network of Data on Environmentally Significant Chemicals (DESCNET).

In view of the large number of potential sources of information, it is imperative that the sources tapped be restricted to those most likely to provide useful data without incurring a major expense for literature searching. The bulk of the needed information could probably be obtained from the sources that were found most useful in SRI's recent (1975) NSF project (see p. 13). In addition, useful data are available in the NIOSH Toxic Substances List, the NLM Toxicology Data Bank (TOXLINE,

---

*Other types of agents would be treated on an ad hoc basis.

CANCERLINE, and so on) and the EPA Oil and Hazardous Material Technical Assistance Data System (TADS).

The relevant data would be provided to the experts in a form similar to that used in the NSF project and they would all be asked to review all of the supplied data in the three areas of product release, environmental transport, and toxic effects, and then provide their estimates of the potential hazard represented by the chemical. This would be done by selecting numbers from a scale such as the following:

Potential Hazard Scale

None	Very Little	Moderate	Major
0	1 2 3	4 5 6 7	8 9 10

Each expert would be asked to supply an estimate for each of the three categories (product release, environmental transport, and toxic effects) and an overall estimate for the chemical. In addition, he would be asked to provide a brief description of the major factors behind each of his four numerical estimates. The contractor would consolidate the separate estimates into a composite estimate for each chemical and prepare descriptions of the major factors behind the composite estimates. In the course of doing this, the contractor would go back to the individual experts to clear up any problems associated with their estimates. If considered desirable, the contractor could point out additional information to experts whose estimates represented extremes and permit them to change their estimates. If funding and time constraints permitted, this process might even be expanded into a formal Delphi technique.

The positive and negative features of the proposed expert-based system are presented in the following table.

EXPERT-BASED SYSTEM

Positive Features	Negative Features
Technically feasible	
Relatively inexpensive	Highly dependent on capabilities of the group of experts
Relatively simple and systematic with built-in checks	Necessarily somewhat subjective
Uses recognized experts (an aid in gaining acceptability to decision makers)	Credibility to various interest groups will depend on experts used
	Consistency over time may be difficult

E. Screening-Indexing System

The preliminary screening-indexing system entailed the computation of indices for release rate, toxicity, and exposure, and the subsequent aggregation of these into a single index for ranking. The perceived advantages of the system were flexibility, simplicity, ease of execution, and explicit statement of assumptions. The principal disadvantages were the subjectivity involved in the selection of weights to be assigned to the components of the toxicity and exposure indices and the equally subjective weighting of interactions between the components of these two indices.

The sections which follow briefly discuss the trade-offs perceived in development of the three indices considered and summarize the recommended strategy.

1. Release Rate Index

Four classes of materials release were recognized, the sum of which equals the total annual release to the environment. These were:

- Emissions and wastes resulting from manufacturing operations, including clean-up, disposal of off-grade batches, and spills.
- Losses during transportation from producer to point of use, including spills, evaporation, and clean-up of shipping containers.
- Dispersive uses (uses in which the chemical or agent is not changed).
- Unintentional production and subsequent loss by combustion, use, or manufacture of other materials.

Quantification of these losses is fairly easy, but the question of whether or not the raw release rates should be transformed by logarithm into an index, to reduce the contribution made by release rates to the ultimate ranking of candidates for STAR documents is not clear. This question is closely related to subjective weightings of mortality and various degrees of morbidity: It is not clear, for example, whether a substance which frequently kills, but is released in small quantities, should have a higher ranking than a less deadly, but more abundant substance; nor is it clear who should make such decisions.

2. Human Toxicity Index

Toxicity in its broadest sense entails a number of negative impacts on individual organisms, including various sources of mortality and forms of morbidity, such as teratogenicity, mutagenicity, allergenicity, and carcinogenicity. Data are commonly available for lethal dosages of various agents, but are slightly less available for indexes of carcinogenicity, mutagenicity, and teratogenicity. Data concerning allergenicity are considerably less common. Similar variations in the availability of data exists for modes of intake, "oral" data being more common than "respiratory" data. The less commonly available data bias the ranking toward the better known agents, but the bias could be appraised, if necessary, by duplicate rankings--one with and one without data other than lethality. Inclusion of all available data requires that the various measures of toxicity be assigned index values to allow for aggregation of data for respiratory and oral ingestion. The method of indexing is unimportant as long as it is coordinated with the release rate index. That is, the ranking of toxicity on a scale of one to ten would make the contribution of toxicity to the ultimate ranking negligible if raw release rate data were used, because of the enormous range ($>10^6$) in the release rates.

Weighting of biological species remained an unsolved problem; the best solution seemed to be to weight nonhuman organisms equally, and to assign man an exceptionally high weight.

3. Environmental Exposure and Damage

Estimates of the transport and accumulation of toxins within the environment are subject to the greatest ambiguity. Rates of physical, chemical, and biological degradation are rarely available and generally are not expressed in forms which permit extrapolation to unstudied environments. Consequently, subjective judgement is both extensive and unavoidable with respect to both the data manipulated and the methods of manipulation, the latter involving questions of weighting of the media through which man and other organisms are exposed, the severity of the environmental damage, and the rapidity of repair.

4. Recommended Strategy

The screening-indexing system proposed in the initial exploration of alternative ranking procedures incorporated three fundamental assumptions:

- Simplicity and ease of execution were of paramount importance.
- Biases should be in the direction of overestimation of hazard if unavoidable.
- In regulatory actions, injury to man generally carries more weight than injury to other organisms and this should be reflected in the screening methodology.

The proposed methodology entailed logarithmic weighting of release rates, the use of all available toxicological data, and differential weighting of media for localized or nonpersistent toxins. For simplicity, it was recommended that index values be assigned to the most hazardous modes of exposure for each toxicological response (such as carcinogenicity) for use in the computation of an aggregate index of toxicity. Differential weighting of media (air, land, water) was recommended on the grounds that the rapidity of immobilization or dilution varies among media, and that the probability of biological contact consequently varies. Nonhuman target organisms were assumed to have equal value and were accordingly weighted inversely by their intrinsic rates of increase, which are an approximation of the ability of these species populations to recover from mass mortality. In routine screening, this methodology ignored impacts on the structure and function of assemblages of organisms; however, provision was made for consideration of these and other impacts that are difficult to appraise, such as aesthetics and population at risk, in the event of ties in the final ranking. It was recommended that the components of each index be aggregated by summation, and that the indices for release rate, human toxicity, and environmental exposure and damage be summed to obtain a final ranking.

F. Model-Based System

The model-based system also defines an environmental hazard index for ranking agents. Ideally, this index is related to the totality of adverse effects on man and his environment that are potentially controllable by EPA. However, to achieve this relationship, it is necessary to subjectively weight various effects. For example, the model system tries to predict the numbers of human cancers, incidences of aesthetic impacts, and percentage of fish killed by an agent; the importance of these three effects are combined by subjective value weights.

The index is computed from a model of the processes that relate the use and occurrence of environmental agents to their end effects. The critical issue in developing such a model is in selecting the important processes and the manner of representing them. For example, a model that ignored toxicity would be useless, but a model that added the half-life to the release rate would be equally unacceptable because it does not represent reality correctly. The selection of processes and representations is subjective, but is also based on the availability of information to carry out the model computations. For example, synergism between two agents, such as between tobacco smoke and asbestos, is clearly important in some cases, but data is so rarely available that the possibility is probably not worth inclusion.

The model includes five basic compartments--source, distribution, fate, effects, and valuation and ranking--related to the ones used in the expert and screening-indexing systems.

The source comparment compares human production (intentional and unintentional) and natural production of the agent.

The distribution compartment examines the uses, unintentional releases, and "ultimate" disposal of the agent, and predicts releases to air, water, and land.

The fate compartment traces the transport of the agent in the environment, accounts for transformations or losses of the agent to inaccessible reservoirs, predicts concentrations in media, and relates this information to the exposure of humans, non-human organisms, and inanimate objects.

The effects compartment develops dose-effects relationships, estimates the dose distribution to populations at risk, and assesses the frequency of various effects as a result.

The valuation and ranking compartment assigns value weights to each effect, derives an aggregate environmental hazard index, and ranks the agent with respect to other agents.

The model-based system is viewed as being outstandingly relevant to the ranking objective; it is relatively objective, explicit, reproducible, robust, and credible. However, it suffers from being less feasible, technically and economically, less acceptable to decision makers, and more complicated and difficult to understand than the other systems.

G. Selection Rationale

Based principally on feasibility, simplicity, and acceptability to decision makers, the expert-based system was selected as the most attractive for further development.

However, it was also recognized that objective information gathering was essential for the credible operation of the expert system. It was seen as desirable that some of this information be presented to the experts in processed rather than (or in addition to) raw form. For example, production, import, export, and intermediate usage information could be combined into a prediction of dispersive use.

This processing can be construed as a more objective portion of the expert system. The model/screening/indexing systems can assist in the determination of what processed information to present.

Because much of the necessary information would be gathered in any case for the expert system, it is possible to operate a parallel "objective"[*] subsystem for only small incremental costs. This subsystem could be used to calibrate the expert results and to identify, for reappraisal, unusual agents that might originally escape attention by the experts.

Consequently, the second phase of the study was directed toward development of a hybrid system based on the expert evaluation of objective data inputs, and supported by an objective subsystem that combined the screening and model systems.

---

[*] The "objective" subsystem is only somewhat "more objective" than the expert system, in that it makes its subjective inputs more explicit.

VI A PRIORITY RANKING SYSTEM BASED ON THE USE OF EXPERT GROUPS

This chapter describes the steps necessary to establish and implement a priority ranking system for evaluating chemicals or groups of chemicals[*] in order to decide which should be the subject of EPA-ORD STAR documents. The proposed system is based primarily on the use of expert groups to review the available data and establish the priorities.

A. Outline of the System

Under the proposed system the EPA contractor would start by gathering available relevant information on the chemical of interest from a selected group of sources and putting it in standardized form for consideration by a committee of nine experts who have been selected on the basis of a preestablished set of criteria. Each expert will be asked to give his individual estimate of the severity of the potential environmental problems associated with each chemical. These estimates will be done on a numerical scale (accompanied by explanatory supporting text) for certain categories of information and on an overall basis for the chemical. These estimates will be combined by an EPA contractor into a composite estimate and accompanying text for submission to a Scientific Review Group which will be asked to review the estimates, examine what is known about feasibility of control, and make recommendations as to the priority of each chemical in the preparation of STAR documents.

---

[*] For agents other than chemicals, or for effects other than biological ones, ad hoc procedures similar to those suggested for the objective subsystem (Chapter VII) would be utilized.

B. Relevant Information and Literature Sources

It is recommended that the information gathered on a particular chemical include selected data elements which:

(1) Identify the pure chemical and the commercial chemical satisfactorily.

(2) Describe the physical and chemical properties of the chemical that are relevant to possible environmental hazard.

(3) Indicate the possible extent of distribution of the chemical to the environment.

(4) Describe the regulation provisions that presently control the release of the chemical to the environment.

(5) Provide information on the major factors involved in the transport and transformation of the chemical in the environment.

(6) Indicate the toxic effects of the chemical on humans and the environment.

Appendix A lists the data elements within these six categories that are recommended for inclusion in the information gathering step. It also indicates the primary sources (publications or organizations) that should be checked, plus a few additional sources for some of the data elements.

Data elements other than those recommended in Appendix A may be of special interest for a particular chemical. Where this is recognized, information on such data elements should be gathered.

C. Format for Presenting Data

It is recommended that the data gathered be presented to the expert committee in the following four categories.

- General data (identification, properties, and regulations).
- Data on distribution to the environment.

- Data on transport and transformations.
- Data on toxic effects.

The recommended detailed format for presenting the information is shown in Appendix B.

D. Composition of the Expert Committee and Criteria for Their Selection

It is recommended that the Expert Committee should consist of nine members. The nine members should be selected to provide three representatives with expertise in each of the following areas of concern:

- The extent of distribution of the chemical to the environment.
- The transport and transformations of the chemical in the environment.
- The toxic effects of the chemical.

To ensure that the desired expertise is actually obtained, it is recommended that the members of the Expert Committee be selected on the basis of the criteria presented in Appendix C. (Although selection of equal numbers of committee members from business, academia, and government may be desirable, it is considered more important to achieve the balance of disciplines outlined in Appendix C.)

E. Operating Procedures

The following procedure is recommended for getting the maximum benefit from the use of the Expert Committee:

- EPA establishes a list of candidate chemicals (or groups of chemicals based on a particular element) and publishes an RFP to obtain a contractor to carry out the contractor tasks described below.

- In cooperation with EPA, the contractor selects a small group (5-10) of chemicals, preferably related in chemical structure, in use pattern, or in toxicology, for consideration by the Expert Committee.
- The EPA contractor collects the relevant data on the selected chemicals from the sources indicated in Appendix A, and puts them into the appropriate format for presentation to the individual members of the Expert Committee (Appendix B).
- Concurrently, the contractor seeks out candidates for the Expert Committee using the recommended criteria (Appendix C) and submits a list to EPA.
- EPA selects candidates from the list and invites them to participate on the committee.
- When the necessary nine members of the Expert Committee have been obtained, the contractor mails the following to the individual committee members:
  - A brief description of the nature of the STAR documents and the expected function of the Expert Committee.
  - The relevant data on the selected chemicals in the prescribed format.
  - An evaluation sheet on which the individual experts can provide their estimates, on a numerical scale, of the severity of the potential environmental problems associated with the chemical. (The recommended form for this evaluation sheet and the details of its use are given in Appendix D.)
- When the composite evaluation sheets have been prepared by the contractor (see Appendix D for details), these are reviewed by EPA.

F. Scientific Review Group Operations

- Concurrently with the processing of the evaluation sheets by the contractor, EPA-ORD establishes a Scientific Review Group whose purpose is to rank in order of priority the list of chemicals evaluated by the Expert Committee, on the basis of the composite evaluation sheets prepared by the contractor.

- The contractor and the chairman of the Scientific Review Group select a mutually satisfactory date for a meeting and the contractor supplies a brief description of the expected function of the group and copies of the composite evaluation sheets to the members approximately 10 days prior to the meeting.
- The chairman establishes the procedure by which the group will rank the chemicals on the list. (It is expected that this will be a system in which each member makes his own ranked list or votes for each chemical separately using some preselected numerical scale.)
- The contractor assists the Scientific Review Group by answering any questions that arise during the meeting, and, as needed, by supplying details of estimates and data in the relevant information summaries submitted to the Expert Committee.
- The chairman of the Review Group submits the priority-ranked list of candidates for STAR documents to EPA-ORD.

G. Estimated Operating Costs

In terms of the number of data elements that could potentially be submitted to the Expert Committee, the system is very ambitious. However, it is recommended that data elements be entered as "NAVA" (not available) whenever a reasonable effort at searching has produced no results. This philosophy allows us to specify a maximum effort for data acquisition which should not be exceeded except for especially significant candidate chemicals.

The costs of operating the expert-based system beyond data acquisition fall into three categories:

- Contractor support activities
- Expert Committee activities
- Scientific Review Group activities.

Estimates of the costs of these activities, as well as those for data acquisition, are shown in Table VI-1. These assume that the experts are able to make their ratings within a period of 20 hours for each group of 10 chemicals, and that only five members of the Scientific Review Group receive travel and consultant fees.

Table VI-1

EXPERT-BASED SYSTEM COSTS
(per chemical)

Activity	Cost Range (dollars)	Average Cost (dollars)
Chemical Identification	$ 50-$ 150	$ 100
Physical-Chemical Properties	50- 150	100
Release and Distribution	200- 600	400
Regulations	100- 300	200
Transport and Transformation	500- 900	700
Toxic Effects	500- 1,100	800
Contractor Support	100- 200	150
Expert Committee	500- 700	600
Scientific Review Group	300- 500	400
Total	$2,300-$4,600	$3,450

Assuming that about 36 chemicals per year are nominated for priority ranking, the system will require about $120,000-$130,000 to operate.

VII DEVELOPMENT OF OBJECTIVE SUBSYSTEM

The objective subsystem is designed to supplement the expert system discussed in the preceding chapter. Basically, it operates on a subset of the information (parameter list) gathered for the experts. However, some information (such as transport in the environmental media) that is left implicit in the expert system must be made explicit in the objective one.

There are two basic components of the objective subsystem: the information gathering component and the information processing component. Although these components generally proceed at the same time, they can be discussed separately.

A. Selection of Parameters

All the parameters of the objective subsystem must be quantifiable in some sense. Even when the basic information is presented as a binary (yes-no) result or as explanatory, the substance must be transformed into a number for use.

In selecting the parameters, we used two criteria. First, the parameter must clearly be of significance to and usable in the information-processing framework of the system (described below). Second, data for a reasonably high percentage of agents must be available in literature sources or obtainable through reasonably simple computations or experiments. Otherwise, the information will not contribute materially to the quality of the ranking. The determination as to whether a given parameter satisfied the first criterion was largely a subjective judgment on our part; the determination as to whether it satisfied the second criterion was made principally on the basis of experience with the parameter in the NSF study.

The parameters selected were classified into three areas--release and distribution, transport and transformation, and effects--similar to those in the expert system. Both of the selection criteria tended to limit the number of parameters in comparison with the expert system. However, more interpretation is needed in using the information associated with the parameters.

The principal parameters for the objective subsystem are listed in Appendix E, with accompanying explanatory texts.

B. Basic System Concepts

The objective subsystem is a hybrid of the screening-indexing and model systems described in Chapter V. The underlying structure is a model of the agent's behavior in the environment, with an environmental hazard index as the output. However, numerous screening questions are asked in the process of exercising the model, and the degree of the model's complexity depends on the answers to them.

In this regard, we have attempted to steer a course between the most common failures of other objective ranking systems. On the one hand, we have attempted to avoid making the system overly complicated when there is little or no data to support such complexities. On the other hand, we have allowed more sophisticated arguments to come into play when information is available to exercise them, thereby avoiding (to some extent) the tendency to oversimplify. For example, intermedia transfers of agents are not addressed by the basic model; however adjustments to model results can be made when intermedia transfer information is known. Our judgments about the relative importance of specific processes and about the complexity or simplicity of the modeling attempts are necessarily *subjective*. *However*, we believe them to be reasonable.

The basic theme of the objective subsystem, like the expert system, is the effects of chemicals on biological systems. This concentration is justified by an examination of the agents that have been selected or suggested for STARs; very few exert their harmful effects in any other ways. However, the subsystem makes ample provision for other conditions. As the prospect of such other conditions occurring becomes less likely, less detail is supplied in the ranking procedure, and more reliance is made on ad hoc procedures. We submit that we cannot build a system that will take care of every eventuality; however, this procedure defines where ingenuity must be exerted or outside help obtained.

C. Development of Procedures

In developing the procedure, we tried to be as explicit as possible in defining the methods for gathering and using information. However, we soon found that this ideal was difficult to achieve, and substantial judgment had to be left to the operators of the system.

The procedure, as developed, consists of a series of steps arranged in branches, only some of which are followed for any one agent. Each step is either a state of information test or an instruction for information processing. Each state of information step leads to one or two or more possible outcome steps, depending on the result of the test. For example, if an agent exerts its effects chemically, then one proceeds down the chemical agent branch, but if not, then one branches off to the nonchemical agent branch. Each information processing step, on the other hand, leads to only one further step, either a test or an instruction.

The overall structure of the procedure is shown in Figure 1. The procedure itself, with further instructions for use, is presented in Appendix F.

D. Operating Personnel and Costs

It was our original hope to construct a procedure that, with the exception of certain ad hoc studies, could be operated by junior-level persons in a near-mechanical fashion. This hope faded, and we now recommend a team with the characteristics shown in Table VII-1. The composition of this team again implies that the "objective" subsystem requiring subjective "expert" opinion, is a hybrid.

The estimated costs of operation of the objective subsystem are shown in Table VII-2. This table assumes that the costs of information gathering for the system parameters will be allocated totally to the operation of the subsystem. In practice, an estimated three quarters of the information gathering costs would be incurred in any case by the operation of the expert system.

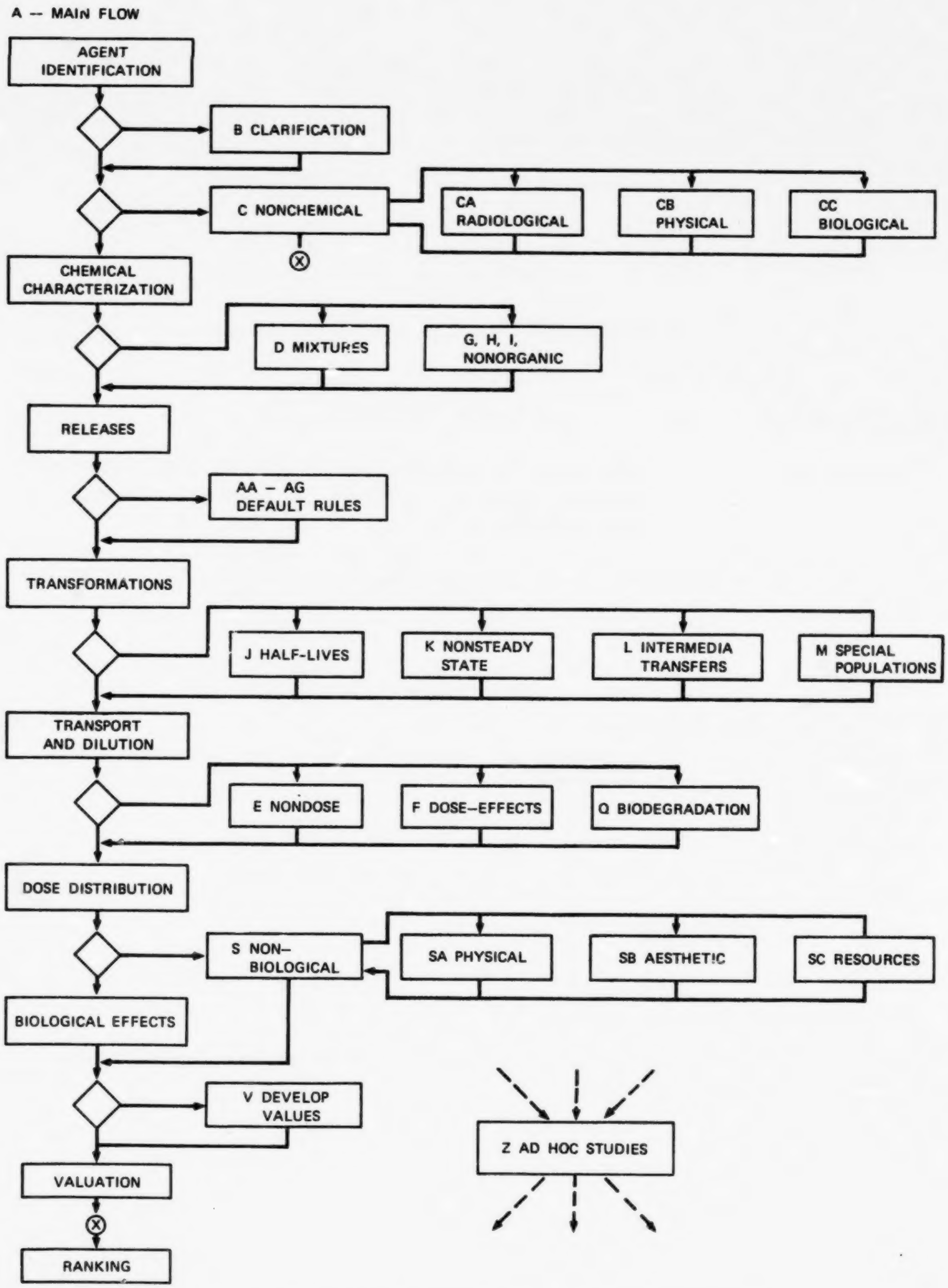

A -- MAIN FLOW
AGENT IDENTIFICATION
B CLARIFICATION
C NONCHEMICAL
CA RADIOLOGICAL
CB PHYSICAL
CC BIOLOGICAL
CHEMICAL CHARACTERIZATION
D MIXTURES
G, H, I, NONORGANIC
RELEASES
AA – AG DEFAULT RULES
TRANSFORMATIONS
J HALF-LIVES
K NONSTEADY STATE
L INTERMEDIA TRANSFERS
M SPECIAL POPULATIONS
TRANSPORT AND DILUTION
E NONDOSE
F DOSE-EFFECTS
Q BIODEGRADATION
DOSE DISTRIBUTION
S NON-BIOLOGICAL
SA PHYSICAL
SB AESTHETIC
SC RESOURCES
BIOLOGICAL EFFECTS
V DEVELOP VALUES
Z AD HOC STUDIES
VALUATION
RANKING

FIGURE 1 OVERALL STRUCTURE OF THE OBJECTIVE PROCEDURE

Table VII-1

PERSONNEL FOR OBJECTIVE SUBSYSTEM

Senior Level

Generalist:	Knowledge of mathematical modeling, environmental science, chemical information, toxic and other effects, and so on
Chemical Economist/ Engineer:	Knowledge of industrial practices and modes of release
Chemist/Kineticist:	Knowledge of physical or physical organic chemistry in real environments
Toxicologist/Health Scientist:	Knowledge of toxic effects in man and nonhuman organisms

Junior Level

Analyst:	General knowledge of literature sources and mathematical techniques
Chemist:	Knowledge of sources for and meaning of chemical parameters
Biologist:	Knowledge of sources for and meaning of biological parameters

Table VII-2

OBJECTIVE SUBSYSTEM COSTS*
(Per Chemical)

Activity	Cost Range (dollars)	Average Cost (dollars)
Gathering Release Information	$ 200-$400	$ 300
Gathering Fate Information	500- 700	600
Gathering Effects Information	450- 600	550
Processing Information and Ranking	400- 600	500
Ad hoc studies	0- 3,000	550
Totals	$1,550-$5,300	2,500

---

*Costs assume that a contractor would operate the system. If operated by EPA in-house, the allocatable costs would be considerably reduced. If the expert system is assumed to be operating and obviating about three-quarters of the information gathering costs, 36 chemicals could be ranked for a marginal cost of about $50,000-$60,000.

Part Three

TEST OF OBJECTIVE SUBSYSTEM

Preceding page blank

VIII DESCRIPTION OF THE TEST

After an extensive review of the recommended expert-based system and its objective subsystem, EPA-ORD decided to test the objective subsystem with a sample of 10 environmental agents of current concern. The full system was not tested because of the expected time required to recruit and orient the two expert groups.

A. Definition of the Agents

A list of candidate agents was received from the technical monitor as part of the Statement of Work. Table VIII-1 shows the list of agents, as defined, and the stated EPA concern leading to their nomination.

Table VIII-1

NOMINATED AGENTS FOR THE TEST

Agent Name	Symbol	EPA Concern
Antimony	Sb	Ocean disposal
Beryllium	Be	Ocean disposal, agricultural runoff
Carbon disulfide	CS_2	Air pollution from energy conversion
Carbonyl sulfide	COS	Air pollution from energy conversion
Cobalt	Co	Drinking water contaminant
Cyanides	CN	General water pollutant, industrial
Heat from manmade sources	Heat	Thermal pollution; system test*
Lithium	Li	Drinking water contaminant
Molybdenum	Mo	Drinking water contaminant
Plutonium	Pu	Radiation; system test*

---

*Chosen to exercise unusual branches of the objective subsystem.

Preceding page blank

The first step in the objective subsystem procedure, as directed by Step A1 (see Appendix F), was to ensure that the agents were well defined. Only CS_2 and COS passed this test unambiguously. The elements (Sb, Be, Co, Li, and Mo) were well defined as such, but conceptually included a wide variety of (mainly inorganic) compounds. To avoid wasting time on unimportant compounds, one to three important representative compounds were selected for each element. In most cases, these compounds were selected to estimate the release and environmental fate parameters of the model, whereas the toxicologically active principle was the element (or its ion) itself. Similar arguments applied to the cyanides, since CN is associated with other chemical species to form molecules. Heat from man-made sources was defined to include waste heat discharged to the environment from the better known sources, such as power generation. Energy from other human activities such as metabolism, end uses of energy, or forest fires was excluded, as were secondary energy effects like changing the albedo of an area of land or removing shade vegetation from the banks of a stream. Only the radiation hazards of Pu were covered, using Pu^{239} as an example. Past releases of Pu from weapons testing, and so on, were excluded. No consideration of the chemical toxicity of Pu was made. Table VIII-2 shows the representative specific agents used and the reasons thereto.

B. Assignment of Tasks

As the interim results of this phase were desired within about 6 weeks of initiation, the subtasks were divided among a rather large group of investigators, larger than would be necessary during normal operations and larger than would be optimal for efficiency. The principal subtasks and responsibilities were:

- Completion of agent identification and preliminary effects checklists, and general literature support (literature specialists)

Table VIII-2

REPRESENTATIVE COMPOUNDS USED

Symbol	Representative(s)	Symbol	Reasons for Selecting Representative
Sb	Antimony trioxide	Sb_2O_3	Commercial significance as fire retardant; high toxicity
Be	Beryllium metal	Be	Primary use as metal
	Beryllium oxide	BeO	Likely end product of many processes; high toxicity
CS_2	As is	--	--
COS	As is	--	--
Co	Cobaltous chloride	$CoCl_2$	Inks, and so on; soluble
	Cobaltous naphthenate	CoNaph*	Paint drier; cobaltous ion is most likely toxic agent
CN	Hydrogen cyanide	HCN	Forms in acid/neutral solutions from other CNs. More toxic than CN^-
	Sodium cyanide	NaCN	Biggest contributor of CN^- ion
	Potassium cyanide	KCN	Second biggest contributor of CN^- ion
Heat	Waste heat	Heat	Convenient definition with respect to reasonable controls
Li	Lithium chloride	LiCl	Drug
	Lithium carbonate	Li_2CO_3	Large commercial use. Both yield Li^+ ion
Mo	Molybdenum trioxide	MoO_3	Important commercially; likely end product
	Molybdenum disulfide	MoS_2	Lubricant
Pu	Plutonium-239 α-radiation	Pu^{239}	Long-lived product of nuclear power industry

---

*A mixture of similar metallo-organic compounds; the symbol is a convenience but is not generally recognized.

- Completion of release worksheets for chemical agents (chemical economists)
- Completion of transport/transformation worksheet (chemists and research analysts)
- Completion of toxicological worksheets (biologists and toxicologists)
- Valuation sensitivity analysis (research analyst)
- Ad hoc study on heat (engineer and ecologist)
- Ad hoc study on Pu (biologist and systems analyst)
- Comprehensive study of CS_2, COS (biologist)
- Integration (project leader).

In accomplishing their tasks, the investigators were asked to:

- Record the steps of the procedure undertaken during their investigations
- Note the areas in which difficulties were encountered and their methods of overcoming or bypassing them
- Comment on opportunities for improving the system to take greater advantage of existing data
- Subjectively evaluate the usefulness and relevance of their activities to the system's objectives
- Comment on the procedures used by other team members.

C. Information Sources

The general philosophy of the STAR ranking system provides that only moderate resources can be devoted to the ranking procedure in comparison with those devoted to the production of STARs. Accordingly, only the most readily available, easily usable, and obvious information sources should be utilized for the ranking, leaving the comprehensive literature search and evaluation for the STAR itself.

There are two general categories of information sources that fit these criteria. First, there are the general information compendia, which provide the same type of information about all, or at least several, of the agents under consideration. These sources should be maintained by the operating system for repeated use at each cycle of ranking. The other category consists of basic documents relevant to a single agent. These basic documents range from treatises on some special aspect, such as chemistry or toxicology, to a complete monograph or criteria document, such as those produced by the National Institute for Occupational Safety and Health, the World Health Organization, or the International Agency for Research on Cancer. This category also includes EPA position papers, preliminary reports, and so on.

Table VIII-3 lists the compendia used in the subsystem test by category of information, and Table VIII-4 lists the basic documents by agent. Complete citations for these references are given in Appendix H.

D. Summary of the Findings

The test proved that it was possible to operate the objective subsystem to the point of computing an environmental hazard index and ranking the agent with respect to those already treated. Furthermore, this procedure consumed only a moderate number of personnel and economic resources,* and was accomplished in a relatively brief timespan. The evaluation of the successes and difficulties of conducting the test is presented in the next chapter.

The results of the test are summarized in Table VIII-5. The rank and environmental hazard index for each agent are shown with a skeletal outline of the reasons for each ranking. The reasons for these rankings are outlined somewhat further in the following summaries for each agent.†

---

*It is estimated that the ranking of 10 agents consumed about $15,000.

†Symbols for representative compounds are shown in parentheses.

Table VIII-3

GENERAL INFORMATION COMPENDIA

Agent Identification and Properties

CHEMLINE
Handbook of Chemistry and Physics (Weast, 1975)
Merck Index (Steiber, 1968)
Lange's Handbook of Chemistry (Dean, 1973)
Encyclopedia of Chemical Technology (Kirk-Othmer, 1963)
"Partition Coefficients and their Uses" (Leo, 1971)

Agent Release

Directory of Chemical Producers (SRI, 1974)
Chemical Economics Handbook (SRI, a)
Census of Manufacturers (Bureau of the Census, 1972)
Mineral Industry Surveys (Bureau of Mines, 1974)
Synthetic Organic Chemicals (International Trade Commission, 1973)
"U.S. Imports, General and Consumption" (Federal Trade Commission, 1973)
"U.S. Foreign Trade, Exports, Commodity by Country" (Federal Trade Commission, 1973a)

Toxicology

TOXLINE
Toxic Substances List (NIOSH, 1974)
Merck Index (Steiber, 1968)
Dangerous Properties of Industrial Materials (Sax, 1975)
Clinical Toxicology of Commercial Products (Gleason, 1969)
"Water Quality Criteria 1972" (EPA, 1972)
Documentation of the Threshold Limit Values (ACGIH, 1971)
Industrial Toxicology (Hamilton, 1974)
Survey of Compounds Which Have Been Tested for Carcinogenic Activity (Shubik, 1940-1973)
Handbook of Poisoning (Dreisbach, 1966)
The Pharmacological Basis of Therapeutics (Goodman, 1970)

Table VIII-4

BASIC DOCUMENTS

Antimony

Chemical Week, Vol. 113, No. 3, 18 July 1973 (Anonymous, 1973)

Behrens and Rosenblatt, *Journal of Chemical Thermodynamics*, Vol. 5, No. 2, March 1973 (Behrens, 1973)

Beryllium

International Agency for Research on Cancer Monograph I (IARC, 1972)

Preliminary Air Pollution Survey of Beryllium and its Compounds (Durocher, 1969)

The Analysts Journal, November 1958 (Boland, 1958)

Beryllium: Its Industrial Hygiene Aspects (Stokinger, 1966)

Reeves, et al., *Cancer Research*, *27*:439 (Reeves, 1967)

Carbon Disulfide

"Carbon Disulfide, Carbonyl Sulfide" (Peyton, 1976)

Characterization of Claus Plant Emissions (Biers, 1973)

"Environmental Aspects of Fossil Fuel Conversion Processes: Liquefaction" (Exxon, 1975)

Assessment of Catalysts for Control of No$_x$ from Stationary Power Plants (Kontsoukos, 1972)

Toxicology of Carbon Disulfide (Teisinger, 1974)

Carbonyl Sulfide

"Carbon Disulfide, Carbonyl Sulfide" (Peyton, 1976)

Characterization of Claus Plant Emissions (Biers, 1973)

"Environmental Aspects of Fossil Fuel Conversion Processes: Liquefaction" (Exxon, 1975)

Matheson Gas Products Information Sheet (Matheson, 1966)

The Chemistry of Carbonyl Sulfide, *Chemical Review*, *57*:621 (Firm, 1957)

Cobalt

Cobalt Monograph (Centre D'Information du Cobalt, 1960)

Table VIII-4 (Concluded)

Cyanide

Handbook of Hazardous Wastes (Capener, 1974)

Heat

Edinger, Duttweiler, and Geyer, *Water Resources Research*, 4:1137, October 1968 (Edinger, 1968)
Edinger, *Water Resources Research*, 6:1392, October 1970 (Edinger, 1970)
Novotny and Krenkel, *Journal Water Pollution Control Federation*, 45: 240, February 1973 (Novotny, 1973)
Biology and Water Pollution Control (Warren, 1971)
Comparative Animal Physiology (Prosser, 1973)
Biology Data Book (Altman, 1974)

Lithium

None

Molybdenum

"Environmental Health Aspects of Selenium, Tellurium, and Molybdenum: A Preliminary Review, No. 3 Molybdenum" (Fishbein, 1974)
"National Emissions Inventory of Sources and Emissions of Molybdenum" (EPA, 1973a)

Plutonium

"Plutonium: Statement of the Problem" (EPA, 1973b)
"An Assessment of Accident Risks in U.S. Commercial Nuclear Power Plants" (USAEC, 1974b)
"Generic Environmental Statement--Mixed Oxide Fuel" (USAEC, 1974a)
Plutonium Information Meeting (Startton, 1974)
"Plutonium and the Other Transuranium Elements" (EPA, 1974)

Table VIII-5

AGENT RANKS AND REASONS

Rank	Agent	Environmental Hazard Index	Dominant Source(s)	Dominant Environmental Process(es)	Dominant Medium	Dominant Effect(s)
1	Cyanides[†]	6×10^6	Plating, other industrial	Precipitation of insoluble compounds	Water	Accidental acute toxicity to man and other organisms
2	Carbon disulfide	4×10^6	Solvents, fumigants	Oxidation	Air	Odor (aesthetic annoyance)
3	Beryllium	5×10^5	Industrial processes	Oxidation; intermedia transfers	Air	Cancer in man
4	Lithium*	2×10^5	Consumer products, e.g., drugs	Water solubility	Water	Central nervous system disorders in man
5	Plutonium	1×10^4	Possibility of accidental release	Intermedia transfers, radioactive decay	Air	Life shortening in man
6	Antimony*	3×10^3	Fire retardants, industrial processes	Intermedia transfers	Water	Heart disease in man
7	Heat	2×10^3	Energy conversion	Dissipation	Water	Fish kill and reproduction loss
8	Carbonyl sulfide*	4×10^2	Sulfur reduction processes	Oxidation	Air	Heart disease in man
9	Molybdenum*	3	Industrial processes	Intermedia transfers	Water	Cattle disease (molybdenosis)
10	Cobalt*	2	Consumer products, e.g., paint	Intermedia transfers	Water	Fish toxicity

---

*These agents all require extreme dose distribution assumptions to exceed threshold. Otherwise, would all rank tied for last with index 0.

†An extreme assumption was also made for cyanides. Without it, CN would have an index of about 10^4 and be tied with plutonium. The resulting ranks would be CS_2, Be, CN + Pu, and Heat.

The backup data and calculations are available for inspection at EPA/ORD and at SRI; Appendix G presents examples of the calculations for cyanides and carbon disulfide.

1. Antimony (Sb_2O_3)

Antimony finds its principal use in alloys with other metals. However, its most important dispersive use is as antimony trioxide, a flame retardant. This compound is assumed to be released to air, water, and land, but to deposit out of the air and to precipitate out of water into sediments and soils. No environmental chemistry is expected. Although toxic effects in fish have been demonstrated, the principal concern is with human inhalation which can lead to severe heart disease. However, only if antimony is concentrated in hot spots will detectable environmental effects be predicted by the subsystem.

2. Beryllium (Be, BeO)

Beryllium is found principally in alloys used by the nuclear and aerospace industries. It is found in rocket exhausts. Beryllium oxide is used in ceramics and glass, and as a catalyst. The oxide is the most likely form of emission from other activities involving beryllium, and is the usual end product of environmental chemistry. It is assumed that the most important releases are to the air, but some releases to other media probably occur. Beryllium also disappears from water and air relatively fast. Berylliosis is a serious concern in occupational settings, but the principal environmental concern is lung cancer. Although beryllium in ambient air is under regulation, the subsystem predicts a considerable hazard still exists.

3. Carbon Disulfide (CS_2)

Carbon disulfide is emitted during its manufacture and during the intermediate production of rayon, cellophane, carbon tetrachloride, and so on. It is dispersively released as a solvent, fumigant, and corrosion inhibitor. Carbon disulfide is produced also in sulfur-reducing technologies such as Claus plants and automotive catalytic converters. It is expected in the effluent of stationary catalytic converters for NO_x control. Carbon disulfide is very volatile and will enter the air, even if discharged to water. In the air, it degrades fairly rapidly to carbonyl sulfide and other products by oxidation. At low concentrations, the principal health effect is increased risk of heart disease. However, the subsystem predicts that the aesthetic impacts from the odor of carbon disulfide would be even more serious overall, putting it high on the list of ten.

4. Carbonyl Sulfide (COS)

Carbonyl sulfide has few commercial uses but is produced in sulfur recovery operations. A gas, it enters the air and is oxidized at moderate rates. Little is known about its toxicity. Even if it is assumed that COS has half the effect of CS_2 with respect to heart disease, and that COS occurs in hot spots, the subsystem still predicts it to be a low hazard chemical.

5. Cobalt ($CoCl_2$, CoNaph)

Cobalt has a number of industrial and consumer uses, and is essential to life as a constituent of vitamin B_{12}. Cobaltous chloride is found in dyes and inks, feed additives, and catalysts. Cobalt naphthenate is a drier for paint. During these dispersive uses CoNaph is assumed to enter air and water as well as to find land disposal. The cobaltous ion is believed to be the environmental form of cobalt normally encountered. Cobalt is assumed to move at moderate rates from air and water to inaccessible reservoirs. Although pneumonitis and dermatitis in man, and losses in domesticated animals and plants are possible, the most likely environmental effect appears to be toxicity to fish, and this occurs only if hot spots of cobalt occur. Thus, cobalt is rated low as a STAR candidate by the subsystem.

6. Cyanides (HCN, KCN, NaCN)

Hydrogen cyanide is used as a fumigant and, more importantly, as an intermediate to organic chemicals such as dyes. The potassium and sodium salts find application in electroplating and other metal treatments, and again as intermediates. HCN enters air and the salts enter water (according to subsystem assumptions), but HCN tends to transfer to water. Cyanides are slowly removed from water by complexation. Their acute toxicity to animal life is well known. It is reasonable to expect occasional fish kills, but effects in man will occur only if there are hot spots. Because of the latter circumstance, cyanides could be a prime STAR candidate.

7. Heat

The forms of waste heat considered to be environmentally damaging come from industry, electric power generation, transportation, and household/commercial sources. Locally, waste heat can raise water temperature a few degrees. Quasi-equilibrium conditions are reached through transfer of heat to the atmosphere. Concentrations of higher-temperature water are more likely in lakes than in rivers. The most likely effects of waste heat are on fish mortality and reproduction. The subsystem predicts that fish mortality is of only moderate concern, and it does not treat reproduction.

8. Lithium (Li_2CO_3, LiCl)

Lithium carbonate (glazes for ceramics, drugs) and lithium chloride (antidepressant drug, heat exchange medium) are two compounds that contribute lithium ion to the nation's waterways, where the ion is believed to remain in solution for long periods of time. Although more severe toxic effects are known, the most likely effects of lithium at environmental levels are central nervous system disturbances. If lithium is found in hot spots, these might place it as a pollutant of moderately high concern.

9. Molybdenum (MoO_3, MoS_2)

The most prevalent molybdenum compounds of human origin are molybdenum disulfide (which is also the ore) and molybdenum trioxide. The sulfide is used as a lubricant and the oxide as a catalyst and in ceramics. Molybdenum metal is used widely in alloys, but most releases would occur in the form of the oxide. It is assumed that molybdenum enters all media, and that it moves rapidly from air and water to inaccessible reservoirs. Various obscure toxic effects are known, of which molybdenosis in ruminants appears the least unlikely at environmental levels. Even if hot spots in agricultural drinking water occur, the subsystem predicts low environmental concern.

10. Plutonium (Pu-239)

EPA concerns about plutonium stem from low level leakage from nuclear fuel reprocessing plants and from the possibility of accidental release of far larger quantities from reactor melt-down. These are future rather than present problems, and the probability of accident appears low. If releases occur, the principal concern would probably be in air, although settling and rainout of the particulate emissions is expected. Inhalation of plutonium can lead to lung and bone cancers and life shortening in man. The subsystem predicts the greater overall harm to be the life shortening and this places plutonium as a pollutant of moderately high concern.

E. Sensitivity Analyses

Two types of sensitivity analyses were conducted in conjunction with the subsystem test. The first type was a formalized procedure to analyze the subsystem's sensitivity to the purely subjective relative value scale for effects. The second set of analyses included a wide range of informal sensitivity tests to variations in assumptions and procedures.

1. Sensitivity to Valuation

In Appendix F it is recommended that the subsystem operator (presumably EPA) develop a set of relative values to be placed on various predicted effects. To provide a starting point, values are suggested for 11 types of effects, relative to an arbitrary value of 1,000 for human mortality, which is expressed in excess deaths per year. No distinction is made for deaths occurring to different age groups or other population categories. However, these values are extremely subjective, and their ratios are probably not transitive. (That is, the ratio of values between deaths and minor illnesses times the ratio of values between minor illnesses and aesthetic impacts is not necessarily equal to the ratio of values between deaths and aesthetic impacts.)

The sensitivity to these value assumptions was tested by defining a range of values for each effect, attempting to reach extreme limits within reason. One other "intermediate" value was suggested in addition to the original ones. These values are listed in Table VIII-6 for the most important effects of the 10 agents ranked.

Table VIII-6

VALUATION RANGE

Effect No.	Effect	Units	Value Per Unit Effect* LO	NOW	ALT	HI
0	Human mortality	deaths/yr	1,000	1,000	1,000	1,000
1	Human morbidity (serious disease)	cases/yr	100	200	300	800
2	Human morbidity (other disease)	cases/yr	5	10	30	100
3	Human life shortening	yr/yr	15	50	50	300
4	Morbidity (domestic animals)	% of pop/yr	50	1,000	300	10,000
5	Mortality (other animals)	% of pop/yr	100	1,000	800	10,000
6	Aesthetic annoyance	occurrences per person/yr	0.01	1	1	50

---

*LO = lowest relative value, NOW = present recommended value, ALT = alternative recommended value, and HI = highest relative value.

Next, several value systems were defined, in which some of the effects took on the high or low extremes. The matrix of these assumptions is shown in Table VIII-7. Using these systems with the values from Table VIII-6 and the predicted numbers of effects, a series of rankings was developed under the various value systems. Both NOW and ALT values were used to fill the blanks in Table VIII-7. The range of rankings achieved for the 10 agents is shown in Table VIII-8. Also shown is the range of rankings most frequently encountered.

Table VIII-7

MATRIX OF VALUE SYSTEMS

Value System	Effect No.					
	1	2	3	4	5	6
"High Death"	LO	LO	LO	LO	LO	LO
"Low Death"	HI	HI	HI	HI	HI	HI
"High Health"	HI	HI	HI			
"Very High Health"	HI	HI	HI	LO	LO	LO
"High Agriculture"				HI		
"Low Agriculture"				LO		
"High Economics"				HI	LO	LO
"Low Economics"						
"High Ecology"					HI	
"Low Ecology"					LO	
"High Aesthetics"				LO	HI	HI
"Low Aesthetics"						LO

Note: Blank elements can be filled either with NOW or ALT.

Table VIII-8

RANGE OF RANKINGS

Agent	Rank	Range of Ranks	Most Frequently Encountered Ranks*
Antimony	6	6-7	6
Beryllium	3	2-4	3-4
Carbon disulfide	2	1-5	2
Carbon sulfide	8	7-8	7-8
Cobalt	10	9-10	9-10
Cyanides	1	1-2	1
Heat	7	5-8	7
Lithium	4	2-4	3
Molybdenum	9	9-10	9-10
Plutonium	5	4-6	5

---

*Incurred for at least 1/3 of the 25 rankings.

From Table VIII-8 it is obvious that the sensitivity to valuation was not particularly great. Half of the agents move through a range of only two places. Three move through only three places, and only one ranges through five. There is little problem in designating cyanides, carbon disulfide, beryllium, and lithium as the top ranking agents.

2. Other Sensitivities

The remaining sensitivities were all tested informally and without conscious effort to test particular assumptions. The only systematic features of these tests were first that plutonium was deliberately ranked by two operators independently and second that all agents were reexamined during final report preparation. The following sensititivies were found:

- To changes in the assumption regarding hot spots. At first, we disregarded any effects when the highest dose calculation did not exceed the stated threshold. Later, we decided to assume that there was some probability of even higher doses occurring and this resulted in a "high dose tail" to the dose distribution. This difference can easily move an agent from the lower half to the upper half of the list, for example, lithium.
- To the choice of effects to be considered. It is essential to identify the "most important" (in terms of largest environmental hazard index) effect. For example, eliminating from consideration the odor effect of carbon disulfide would move it from the top of the list to the bottom.
- To consideration of all sources of release. Sometimes it is possible to miss an important release, for example, from combustion. This can make a difference of several orders of magnitude in ranking index (although usually it does not). The resulting differences in rank may be several places, but rarely involve a movement from bottom to top or vice versa.
- To interpretation of toxicology. Toxicology is frequently very qualitative, and it is rare for more than two points on a dose-response curve to be known. The subsystem's sensitivity to the assumption of a threshold or no

threshold is similar to its sensitivity for hot spots. On the other hand, sensitivity to changes in curve shape not involving threshold shifts is not very great.

- To errors. When one is dealing with a complex series of computations, it is relatively easy to make a mistake that is not readily spotted by a checker. Obviously, the significance of an error depends on its magnitude, but errors of less than an order of magnitude tend to be relatively unimportant to the rankings.

In summary, the objective subsystem is sensitive to changes in assumptions, but much less sensitive than one might assume from the degree of uncertainty expected.

IX EVALUATION OF THE TEST

A. Criteria for Evaluation

The objective subsystem can be judged by the same criteria used to select among alternative ranking systems in the original development phase. These criteria (the first five of which are considered somewhat more important than the last four) were:

Technical feasibility
Economic feasibility
Acceptability to decision makers
Robustness with respect to uncertain information
Simplicity and understandability
Credibility to various interest groups
(Relative) objectivity
(Relative) explicitness
Reproducibility and traceability

The degree to which the test addressed these criteria and the success of the objective subsystem in satisfying them are discussed below; associated issues are also raised and evaluated.

B. Successes and Failures of the System

1. Technical Feasibility

The system proved workable in an overall sense. No insurmountable difficulty was encountered that prevented the team from deriving an environmental hazard index for the purpose of ranking. However, the information desired by the system was often lacking or highly uncertain; reliance on default values or assumptions occurred far too frequently for comfort. Moreover, the procedures were ill-defined at points, and the analyst had to provide his own interpretation.

The technical difficulties of greatest concern seem to fall in the following areas:

- Release factors--The fraction of processed materials released by industry and the fraction of consumer products reaching various media usually are not known, and need to be estimated by default procedures. The need for changes in the default procedures also seems to be indicated.
- Persistence and intermedia transfer--Environmental transformations of compounds are difficult to predict, especially for inorganics; intermedia transfers seem to be more important than they were originally thought to be, however, data are scanty and a more robust procedure is needed.
- Transport and diffusion--Virtually no information on transport and diffusion seems readily available, and computations are suspect; however, verifiable predictions were surprisingly accurate (well within the correct order of magnitude).
- Populations at risk--This feature has not been adequately worked out; geographical descriptions were the only ones easily associated with the agents.
- Toxicology interpretation--Although the basic toxicology was usually available, the interpretation of the information into quantitative terms was fraught with uncertainty. In addition, extreme assumptions about the distribution of doses were necessary to predict effects above threshold for half of the agents.

In general, the technical feasibility of the subsystem seems to depend on the creativity and boldness of the operator in dealing with deficiencies in information and with subtleties of procedure not treated in detail by the system instructions. This observation implies that the principal operator should be a good generalist on the environment, with considerable ability in making educated guesses.

2. Economic Feasibility

The subsystem proved perhaps even more economically feasible than anticipated. Data gathering required an average of about 40 hours of (mainly) junior professional effort per agent. Ranking required approximately 8 hours of senior professional time per agent. Consequently, the basic test required about $1,500 per agent. Of course, many of the deficiencies in technical feasibility result from the decision not to devote more financial resources, so these two criteria trade-off against one another.

3. Acceptability to Decisionmakers

This criterion for the system has yet to be tested.

4. Robustness

The subsystem provides default values for many of its parameters, and is robust in this sense. However, many inputs require subjective evaluation of scanty or missing information. The treatment of these inputs is sometimes critical to the overall ranking. However, uncertainties rarely changed ranks by more than three places out of ten.

5. Simplicity and Understandability

The subsystem is quite complex from the point of view of even a scientifically oriented layman. Many of the procedures, especially the default steps, need to be taken on faith as they are not explained in any detail. However, the steps do make sense if closely examined.

6. Credibility

This criterion for the system has not been tested. The complexity could deter credibility in skeptics, but enhance it for others.

Although credibility to the operators of the system is not a necessary criterion, most of the operators felt extremely uneasy in making the assumptions, extrapolations, and interpretations of minimal information that are necessary for the system operation. The system is probably less credible to the operator than to outside evaluators.

7. Objectivity

The subsystem is relatively objective in comparison with most other priority systems. However, it required more subjective inputs than were expected before the test. Some of the subjective features are:

- Choice of the processes in the real world to model in the system.
- Default values and procedures.
- Interpretation of conflicting, incomplete, or missing information, especially in
  - toxicology
  - release factors
  - intermedia transfers.
- Choice of effects to consider.
- Treatment of agents which showed doses below threshold on the first computation of effects. In these cases we made an assumption on the distribution of higher doses so that the threshold was exceeded by at least some doses.

8. Explicitness

Most of the reasoning in the subsystem is relatively explicit and can be examined on the worksheets and accompanying notes. However, time and space limitations prevented our making all assumptions explicit.

9. Reproducibility and Traceability

The system was designed to be traceable by worksheets and other reports. Except for the occasional lack of explicitness in assumptions, cited above, the system succeeds in this design. However, it is not as reproducible as hoped because of the subjectivity mentioned earlier. Both ranking by different persons and ranking at different times by the same person gave different answers, sometimes by orders of magnitude.

10. Summary Statement

In general, however, the subsystem adequately meets the criteria more often than not. Consequently, it should be considered a valuable procedure in the systematic setting of priorities for STARs. It is particularly good at outlining a comprehensive picture of an agent's total behavior in the environment; for example the subsystem identifies factors that limit the agent's potential for environmental harm (e.g., short half-life) and highlights areas of great uncertainty that are critical to understanding that potential. Nevertheless, the subsystem's deficiencies are sufficiently disturbing that the rankings it produces should be carefully examined before decisions to undertake STARs are made. In essence, this conclusion is consistent with the previous recommendation to use the objective subsystem only as an input to and monitor of an expert system of STAR selection.

C. Suggested Improvements

In the course of operating the subsystem, many areas of needed improvement were identified. These ranged from the correction of typographic errors to the addition of major branches. Not all of these improvements were clearly economically justified. We list below the improvements most likely to be worth their cost, with the additional observation that every new agent put through the system will probably generate additional modifications, and a continuous improvement should be expected with use of the subsystem.

A group of simple improvements have already been incorporated into the subsystem and are therefore not detailed here. Recommended further improvements fall into three groups. The first group could be incorporated with relatively little additional effort:

- Development of an explicit procedure for handling subthreshold effects predictions, or for assuming a high-dose distribution (this might not be an acceptable improvement to certain philosophical/scientific attitudes). A proposed procedure is included in Appendix F.
- Revision of procedures for inorganic compounds to make these procedures parallel to those for organic chemicals.
- Revision and expansion of the procedures for treating nonsteady-state conditions (Branch K). Some revisions have already been made.

The second group could be accomplished with modest effort:

- Provision of explicit instructions and worksheets for describing populations at risk. (See Worksheet A37 in Appendix F. This worksheet was not used in the test.)
- Provision of explicit instructions and worksheets for describing geographical concentrations of exposure. (See Worksheet A22 in Appendix F. This worksheet was not used in the test.)

The third group would require somewhat more effort:

- Addition of a set of procedures for dealing with ocean and/or estuarine pollution such as river runoff, precipitation, and dumping. The National Academy of Sciences publication* is recommended as a guide.

---

*Assessing Potential Ocean Pollutants (NAS, 1975a).

- Addition of a methodology for land contamination and effects (including direct exposures and transfers to ground and surface water), for use with pesticides and similar materials.
- Expansion of the procedure for dealing with transportation releases and other spills, using Office of Hazardous Materials techniques. Alternatively, drop transportation branch as unworkable and under the responsibility of the Department of Transportation.

Appendix A

DATA ELEMENTS FOR THE EXPERT SYSTEM

Preceding page blank

Appendix A[*†]

DATA ELEMENTS FOR THE EXPERT SYSTEM

Data Element	Primary Source	Other Sources
I Data Elements Needed to Identify the Pure Chemical and the Commercial Chemical		
1. Chemical Abstracts Services Registry Number	CHEMLINE	TADS, TSL
2. Molecular formula	CHEMLINE	TADS, TSL
3. Structural diagram	Merck	SOCMA
4. Synonyms	CHEMLINE	TADS, TSL
5. Trade names for commercial chemical	CHEMLINE	TSL, NIOSH, CPSC FDA, EPA-OPP
6. Composition of commercial chemical	Product Bulletins	NIOSH, CEH
II Data Elements Needed to Describe Physical and Chemical Properties Relevant to Possible Environmental Hazard		
7. Melting point	TDB	TADS, HPC
8. Vapor pressure	TDB	HPC
9. Boiling point	TDB	TADS, FPG, HPD
10. Decomposition point	HPC	TADS
11. Combustion products	TADS	
12. Flash point	TDB	TADS, FPG, HPC
13. Density	TDB	TADS, HPC, FPG
14. Flammability limits	TADS	FPG
15. Explosive limits	TADS	
16. Solubility in water	TDB	TADS, HPC
17. Solubility in nonpolar solvents	TDB	TADS, HPC

---

[*] Source abbreviations used in this section are explained in Appendix I.

[†] See Appendix F for nonchemical agents and nonbiological effects.

Preceding page blank

Data Element	Primary Source	Other Sources
III Data Elements Needed on Regulations that Control the Release of the Chemical to the Environment		
18. Environmental Regulations		
a. Effluent limitations guidelines for 30 industries (water pollution)	EPA-OWHM	
b. Pollutant discharge permits (water pollution)	EPA-OEGC	
c. Toxic pollutants standards (water pollution)	EPA-OWHM	
d. Hazardous substances standards (water pollution)	EPA-OWHM	
e. Drinking water standards	EPA-OWHM	
f. Ocean disposal regulations	EPA-OWHM	
g. Toxic substances regulations*	EPA-OTS	
h. Pesticide registration regulations	EPA-OPP	
i. Pesticide residue tolerances	EPA-OPP	
j. Ambient air quality standards	EPA-OAWM	
k. Emission standards	EPA-OAWM	
l. Solid waste regulations*	EPA-OSWMP	
19. Meat additive regulations	USDA-MID	
20. FDA Regulations		
a. Food additive regulations	FDA	
b. Cosmetics regulations	FDA	
c. Drug regulations	FDA	
21. Transportation regulations	DOT and USCG	
22. Consumer product safety regulations	CPSC	
23. Occupational safety and health regulations	OSHA	
IV Data Elements Needed to Indicate Possible Extent of Distribution of the Chemical to the Environment		
24. Annual U.S. production (P)	SOC (organics) COM (inorganics)	CEH MY
25. Percent losses during manufacture (F_{PL})	Industry survey	
26. Estimated annual losses during manufacture	$P(F_{PL})$	

---

*Regulations are pending.

	Data Element	Primary Source	Other Sources
27.	Annual U.S. imports (I)	FT-246	IBCP
28.	Annual U.S. exports (E)	FT 410	
29.	Apparent U.S. consumption (C)	$C = P + I - E$	
30.	Percent of consumption to dispersive uses (F_D)	CEH	
31.	Estimated annual dispersive uses	$C(F_D)$	
32.	Release rate (R)	$R = P(F_{PL}) + C(F_D)$	
33.	Pollution Control		
	a. Air pollution controls used at producing plants	Industry survey	EPA-OAWM
	b. Water pollution controls used at producing plants	Industry survey	EPA-OWHM
34.	Principal transportation methods	DOT	TADS
35.	Estimated losses during transportation	DOT	TADS
36.	Consumption pattern (amount to various uses)	CEH	
37.	Disposal methods following major uses	EPA (several program offices)	Industry associations

Data Elements Needed on Major Factors Involved in the Transport and Transformation of the Chemical in the Environment

38.	Octanol-water partition coefficient	CR	CA
39.	Biochemical oxygen demand	JWPCF	EPA (various program offices)
40.	Chemical oxygen demand	JWPCF	EPA (various program offices)
41.	Rate of oxidation in air and water	Calculation by expert from literature data	
42.	Hydrolysis rate (pH 7 at 20°-25°C)	CA	Calculation by expert from literature data
43.	Concentrations in environmental media (air, water, land, sediments)	TDB	TADS, STORET, SAROAD
44.	Concentrations in organisms (fish, mammals, birds, insects, micro-organisms, plants)	TADS	BA
45.	Uptake rates by environmental media	TOXLINE	BA
46.	Uptake rates by organisms	TOXLINE	BA
47.	Release rates for environmental media	TOXLINE	BA
48.	Release rates for organisms	TOXLINE	
49.	Residence times in environmental media	TADS	STORET, SAROAD

Data Element	Primary Source	Other Sources
50. Residence times in organisms	TOXLINE	BA
51. Ratio of concentrations in organisms to concentrations in pertinent environmental media	TDB	TOXLINE, BA
52. Mode of entry to organisms (oral, respiratory, dermal)	BA	CA
53. Site of storage in organisms (organs, tissues, and fluids)	TDB	BA, CA
54. Mode of release by organisms	TDB	BA, CA
55. Biodegradation products (metabolites) of the chemical in organisms	TDB	BA, CA, MP
VI Data Elements Needed on Toxic Effects of the Chemical		
56. Animal Effects		
a. LD50, LC50	TDB	TOXLINE, TMIC
Target organs in mortality	TOXLINE	MEDLINE, TMIC
b. LDLo (acute, subchronic, and chronic)	TOXLINE	MEDLINE, TMIC
Clinical observations of toxic effects (acute, subchronic, and chronic)	TOXLINE	MEDLINE, TMIC
c. Metabolic effects indicative of disease	MEDLINE	BA
57. Human Effects		
a. Excess mortality from acute or episodic exposures	TOXLINE	MEDLINE, TMIC
b. Excess mortality from chronic exposures	TOXLINE	MEDLINE, TMIC
c. Threshold limit values or no effects thresholds for acute effects	TSL	TOXLINE
d. Threshold limit values or no effects thresholds for chronic effects	TSL	TOXLINE
Clinical observations of toxic effects (acute, subchronic, and chronic)	TOXLINE	
e. Metabolic effects indicative of disease	MEDLINE	MEDLINE, TMIC
58. Other Data (for inclusion if ascertained in the course of searching for the above information)		
a. Significant interactions (for example, antagonism, synergism) with other agents in either animals or humans	TOXLINE	MEDLINE, TMIC
b. Dose-response data	TOXLINE	MEDLINE, TMIC

Appendix B

RECOMMENDED FORMAT FOR PRESENTING DATA TO THE EXPERT COMMITTEE

Appendix B

RECOMMENDED FORMAT FOR PRESENTING DATA TO THE EXPERT COMMITTEE[*]

I General Identification Data

1. CAS No.: ________ 2. Molecular formula: __________

3. Structural diagram:

4. Synonyms:

_______________ _______________ _______________
_______________ _______________ _______________
_______________ _______________ _______________
_______________ _______________ _______________
_______________ _______________ _______________
_______________ _______________ _______________

5. Trade names for commercial chemicals:

_________________ _________________ _________________
_________________ _________________ _________________
_________________ _________________ _________________
_________________ _________________ _________________
_________________ _________________ _________________

---

[*] Listed in the same order as in Appendix A; the reasons for seeking these data and possible sources are also shown in Appendix A.

6. Composition of commercial chemical:

% active ingredient:

% and name of major impurities:

Content and names of minor impurities:

__________ (%, ppm, ppb) __________

__________ (%, ppm, ppb) __________

II Physical and Chemical Properties

7. Melting point: _____°C

8. Vapor pressure: _____mmHg at _____°C

9. Boiling point: _____°C at _____mmHg

10. Decomposition point: _____°C

11. Combustion products:

Major	Minor

12. Flash point: _____°C 13. Density: _____g/cc at _____°C

14. Flammability limits: _____% - _____% by volume in air

15. Explosive limits: _____% - _____% by volume in air

16. Solubility in water: _____ parts in 100 parts at _____°C

17. Solubility in nonpolar solvents: _____ parts in 100 parts at _____°C

III Regulations

18. EPA guidelines, standards, and regulations
    a. Effluent limitations guidelines
        i) for the industries producing most of the chemical:

        ii) for the industries using most of the chemical:

    b. Pollutant discharge permits issued for the chemical:
        i) to producing companies

        ii) to consuming companies

    c. Toxic pollutants:

    d. Hazardous substances:

    e. Drinking water:

    f. Ocean disposal:

    g. Toxic substances:

    h. Pesticide registration:

    i. Pesticide residue tolerances:

    j. Ambient air quality:

    k. Emissions:

    l. Solid wastes:

19. USDA meat additive regulations

20. FDA regulations

    a. Food additives:

    b. Cosmetics:

    c. Drugs:

21. Transportation regulations

    a. DOT regulations:

    b. USCG regulations:

22. Consumer product safety regulations:

23. Occupational safety and health regulations:

IV Data on Distribution to the Environment

24. Annual U.S. production (P): ______Kg
25. Percent losses during manufacture (F_{PL}): ______%
26. Estimated annual losses during manufacture (PxF_{PL}) ______Kg
27. Annual U.S. imports (I): ______Kg
28. Annual U.S. exports (E): ______Kg
29. Apparent U.S. consumption ($C = P + I - E$): ______Kg
30. Percent of consumption to dispersive uses (F_D): ______%
31. Estimated annual dispersive uses (CxF_D): ______Kg
32. Release rate ($R = PxF_{PL} + CxF_D$): ______Kg

33. Controls used at producing plants

    a. for air pollution:

    b. for water pollution:

34. Principal transportation methods:

35. Estimated losses during transportation: ______Kg

36. Consumption pattern

Use	% of Total Consumption

37. Disposal methods following major uses

Use	Disposal Method

V Data on Transport and Transformation

38. Octanol-water partition coefficient:

39. Biochemical oxygen demand (BOD):

40. Chemical oxygen demand (COD):

41. Rate of oxidation in air and water:

42. Hydrolysis rate (pH 7):

43. Concentrations in environmental media

Medium	Concentration	Units
Air	____________	_____
Water	____________	_____
Land	____________	_____
Sediments	____________	_____

44. Concentrations in organisms

Organisms	Concentration	Units
________	____________	_____
________	____________	_____
________	____________	_____
________	____________	_____

45. Uptake rates by environmental media

Medium	Uptake Rate	Units
Air		
Water		
Land		
Sediments		

46. Uptake rates by organisms

Organisms	Uptake Rate	Units

47. Release rates for environmental media

Medium	Release Rate	Units
Air		
Water		
Land		
Sediments		

48. Release rates for organisms

Organisms	Release Rate	Units

49. Residence times in environmental media

Medium	Residence Time	Units
Air		
Water		
Land		
Sediments		

50. Residence times in organisms

Organism	Residence Time	Units

51. Ratio of concentrations in organisms to those in media

Organism/Medium	Ratio of concentration

52. Mode of entry to organisms

Organism	Mode of entry (oral, respiratory, dermal)

53. Site of storage in organisms

Organism	Site of storage (organs, tissues, and fluids)

54. Mode of release by organisms:

55. Biodegradation products (metabolites) in organisms

Organism	Biodegradation Products

VI Data on Toxic Effects

56. Animal Effects

a. Mortality

LD50: ______mg/Kg

Animal species:

Route of administration:

Gross pathology of principal target organs:

Microscopic pathology of principal target organ:

LC50: ______mg/m^3

Animal species:

Calculated total dose (mg/m^3 x time x intake rate):

Gross pathology of principal target organ:

Microscopic pathology of principal target organ:

b. Morbidity

Acute effects

LDLo: ______mg/Kg

Animal species:

Route of administration:

Clinical observations:

Subchronic effects

LDLo: ______mg/Kg

Animal species:

Route of administration:

Clinical observations:

Chronic effects

LDLo: ______mg/Kg

Animal species:

Route of administration:

Clinical observations:

c. Metabolic effects indicative of disease

LDLo: ______mg/Kg

Animal species:

Route of administration:

Metabolic effects:

57. Human Effects

a. Excess mortality from acute exposures

occupational groups:
route of exposure:
excess mortality:
pathology of principal target organs:

general population:
route of exposure:
excess mortality:
pathology of principal target organs:

selectively vulnerable subgroups:
route of exposure:
excess mortality:
pathology of principal target organs:

b. Excess mortality from chronic exposures

occupational groups:
route of exposure:
excess mortality:
pathology of principal target organ:

general population:

route of exposure:

excess mortality:

pathology of principal target organ:

selectively vulnerable subgroups:

route of exposure:

excess mortality:

pathology of principal target organs:

c. Threshold limit value (TLV) or no effects threshold (NET) from acute exposures

occupational groups:

route of exposure:

TLV or NET:

clinical observations:

general population:

route of exposure:

TLV or NET:

clinical observations:

selectively vulnerable subgroups:

route of exposure:

TLV or NET:

clinical observations:

d. Threshold limit value (TLV) or no effects threshold (NET) from chronic exposures

occupational groups:

route of exposure:

TLV or NET:

clinical observations:

general population:

route of exposure:

TLV or NET:

clinical observations:

selectively vulnerable subgroups:

route of exposure:

TLV or NET:

clinical observations:

e. Metabolic effects indicative of disease

population exposed:

route of exposure:

TLV or NET:

metabolic effects:

58. Other Data

a. Significant interactions with other agents

(1) In animals

other agents:

animal species:

route of exposure:

clinical observations:

(2) In humans

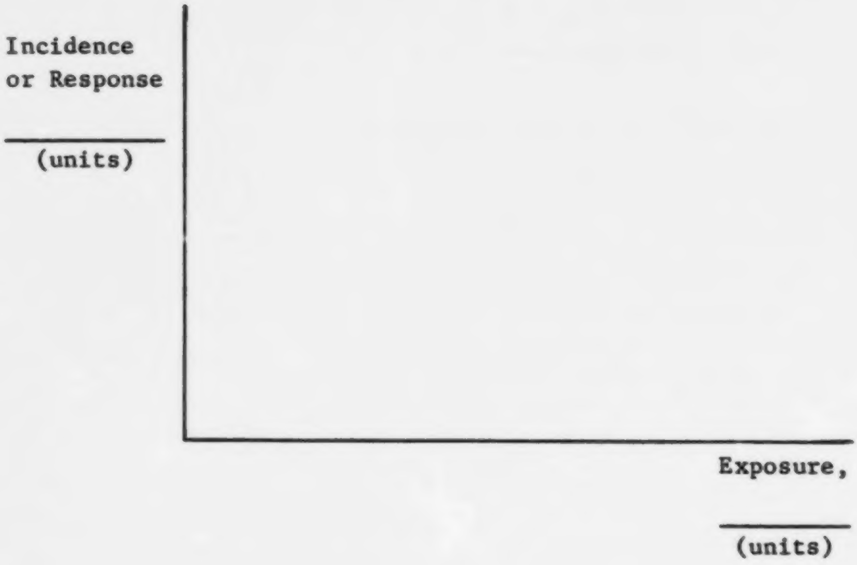
other agents:

population exposed:

route of exposure:

clinical observations:

b. Dose-response data



Appendix C

RECOMMENDED CRITERIA FOR SELECTING MEMBERS OF THE EXPERT COMMITTEE

Appendix C

RECOMMENDED CRITERIA FOR SELECTING MEMBERS OF THE EXPERT COMMITTEE

I Experts on the Extent of Distribution of the Chemical to the Environment

Chemical Market Research

Academic Training	Master's degree in chemistry or chemical engineering. Bachelor's degree in these disciplines plus a Master's degree in business administration. Experience equivalent to these degrees would also be satisfactory.
Relevant Experience	A minimum of 10 years experience, the last 5 of which have been in the area of chemical market research on the chemical (or group of chemicals) of concern.
Peer Recognition	Membership in a principal scientific society representing candidate's discipline, preferably the Chemical Market Research Association. Publication, during the last 5 years, of at least one article (in an industry-oriented periodical, encyclopedia, or book) on the chemical (or group of chemicals) of concern.

Preceding page blank

II Experts on the Transport and Transformations of the Chemical in the Environment

Environmental Engineering

Academic Training	Either a Ph.D., Sc.D., or equivalent experience in an engineering discipline related to pollution control.
Relevant Experience	A minimum of 10 years experience, the last 5 of which have been in the area of research, development, or teaching of pollution control.
Peer Recognition	Membership in a principal scientific society representing candidate's discipline. Publication of at least 10 papers in refereed journals in the related field since completion of academic training.

Ecology, Earth, and Life Sciences

Academic Training	Either a Ph.D., Sc.D., or equivalent experience in the subdisciplines of aquatic or terrestrial ecology, which include fisheries, limnology, botany, geology, meteorology, and oceanography.
Relevant Experience	A minimum of 10 years experience, the last 5 of which have been in the area of environmental pollutant transport, ecological effects of pollutants, and/or environmental impacts of pollutants.
Peer Recognition	Membership in a principal scientific society representing candidate's discipline. Publication of at least 10 papers in refereed journals in the related field since completion of academic training.

Environmental Health

Academic Training	Either a Ph.D., Sc.D., M.D., or equivalent experience in environmental health, public health, industrial hygiene, or epidemiology.
Relevant Experience	A minimum of 10 years experience, the last 5 of which have been in the areas of pollutant transport, transformations, exposure and/or health effects. An interdisciplinary background covering pollution control, ecology, and health effects is desirable.
Peer Recognition	Membership in a principal scientific society representing candidate's discipline. Publication of at least 10 papers in refereed journals in the related field since completion of academic training.

III Experts on the Toxic Effects of the Chemical

Animal Toxicology

Academic Training	Either a Ph.D., Sc.D., D.V.M., M.D., or equivalent experience in toxicology, pharmacology, pathology, biochemistry, or medicine.
Relevant Experience	A minimum of 10 years experience, the last 5 of which have been in the area of toxicology of environmental pollutants or xenobiotics.
Peer Recognition	Membership in the principal scientific society representing candidate's discipline. Publication of at least 10 papers in refereed journals in the related field since completion of academic training.

Human Toxicology

Academic Training	Either a Ph.D., Sc.D., M.D., or equivalent experience in epidemiology or occupational medicine.
Relevant Experience	A minimum of 10 years experience, the last 5 of which have been in the area of epidemiology of environmental pollutants or xenobiotics.
Peer Recognition	Membership in the principal scientific society representing candidate's discipline. Publication of at least 10 papers in refereed journals in the related field since completion of academic training.

Appendix D

RECOMMENDED EVALUATION SHEET AND PROPOSED METHOD OF USE BY MEMBERS OF THE EXPERT COMMITTEE

Appendix D

RECOMMENDED EVALUATION SHEET AND PROPOSED METHOD OF USE BY MEMBERS OF THE EXPERT COMMITTEE

The Evaluation Sheet submitted for each chemical to all nine members of a particular Expert Committee would have the following format:

Evaluation Sheet for Estimating the Severity of the Potential Environmental Problem Associated with the Chemical

Please circle the number which most closely represents your estimate of the chemical's environmental significance in the following four categories and provide a short description of the major factors behind each of your four estimates.

1. Estimate the significance of distribution of the chemical to the environment.

POTENTIAL PROBLEM SCALE

None	Very Little	Moderate	Major
0	1 2 3	4 5 6 7	8 9 10

Major factors involved:

Preceding page blank

2. Estimate the significance of transport and transformations of the chemical in the environment.

POTENTIAL PROBLEM SCALE

None	Very Little	Moderate	Major
0	1 2 3	4 5 6 7	8 9 10

Major factors involved:

3. Estimate the significance of the chemical's toxic effects.

POTENTIAL PROBLEM SCALE

None	Very Little	Moderate	Major
0	1 2 3	4 5 6 7	8 9 10

Major factors involved:

4. Estimate the overall severity of the potential environmental problem associated with the chemical.

POTENTIAL PROBLEM SCALE

None	Very Little	Moderate	Major
0	1 2 3	4 5 6 7	8 9 10

Major factors involved:

It is recommended that the contractor process these evaluation sheets in the following way upon receipt from the members of the Expert Committee:

1. Review the estimates for instances in which one expert's estimate and major factors differ markedly from the information supplied by the other experts. Telephone this

expert to point out the difference and ask him to consider changing his estimate or to provide more information if he feels a change is not appropriate. In the latter case, the information provided should be telephoned to the other experts and they should be given an opportunity to change their estimates.

2. Once the estimates have been finalized, compile a composite evaluation sheet for each chemical by averaging the estimates from the nine experts in each of the four categories, and prepare a description of the major factors involved using the descriptions provided by the experts as guidance.

3. Select one of the chemicals from those considered by the first Expert Committee for submission to subsequent Expert Committees along with the new chemicals submitted to these committees. The estimates on the composite evaluation sheet for this chemical can then be compared with the estimates from the subsequent committees and used to maintain consistency across the estimates submitted at different times. If the composite estimates for the reference chemical from a particular committee vary widely from the original estimates, then the composite estimates for the new chemicals in the group considered by the new committee may need to be adjusted accordingly.

Appendix E

PARAMETERS FOR USE IN THE OBJECTIVE SUBSYSTEM

Preceding page blank

Appendix E

PARAMETERS FOR USE IN THE OBJECTIVE SUBSYSTEM

Three team members were asked to recommend parameters for inclusion in the objective subsystem, using as criteria (1) that data for the parameters should be available for a substantial fraction of the agents and (2) that the parameter have reasonably high relevance to the prediction of environmental effects from controllable sources of the agent.

This appendix presents the rationale behind the team members' selection of parameters in the categories of release, fate, and effects in the environment. It also presents the rationale behind modifications introduced to weave the parameters into a mathematical model.

I Release to the Environment

The processes and uses that can lead to the release of pollutants to the environment were identified (Table E-1) as a first step in refining parameters, defining source data, and selecting standard units for parameters for such releases. No attempt was made to develop equations that would sum the listed routes of release.

Availability of data related to all Table E-1 release routes A-N would be the best possible case for summarizing quantitative information for priority ranking decisions; Table E-2 describes parameters, symbols, and information sources for these routes. The information source listings are probably not all-inclusive and could be developed further.

Tables E-1 and E-2 represent the level of detail that might be required for assessment of a group of "critical" chemicals. However, for practical reasons it may not be reasonable to go to this level of detail.

Preceding page blank

Table E-1

PROCESSES AND USES LEADING TO RELEASE OF POLLUTANTS TO THE ENVIRONMENT

Activity	Description of Release Routes to Environment	Symbol
Manufacture	"Normal" emissions or waste disposal during manufacturing process, including clean-up	A
	Off-grade batch disposal	B
	Accidental plant release (spills, and so on)	C
	Release or waste from cleaning of bulk storage facilities	D
Transportation of Material	Release during loading--spills, evaporation	E
	Release during transport	F
	Release during unloading--spills, evaporation	G
	Release during clean-up of shipping container	H
Direct Dispersive Use (not formulated w/other materials)	Direct release related to method of use	I
	"Sealed" dispersive use	J
Intermediate Use	Loss during conversion to another material (includes storage, transfer, processing at conversion site)	K
↕ Interrelated		
Release as By-Product or Impurity (in manufacturing of other product)		A-D Apply with quantities at much lower levels
Formulated Product Use	Release during storage, transfer and formulation	L
	Release during use of the formulated product	M
Nonintentional Production	Nonintentional, nonmanufacturing release via chemical or physical processes	N

Table E-2

DATA SOURCES AND UNITS FOR RELEASE ROUTES A-N

Release Route Symbol	"Published" Data Sources/Units	"Other" Data Sources/Units
A	1) NSF (Organic Chemicals); (kg/yr) 2) EPA documents; (kg/yr) 3) NIOSH (kg/yr)	1) Industrial survey; kg/yr or % of production (P) 2) Expert estimate; (% of P in kg/yr)
B		Same as A
C		Same as A
D		Same as A
E		Same as A
F	1) Department of Transportation (DOT)	1) and 2) same as A 3) Survey of shippers; % of quantity shipped in kg/yr)
G		1), 2) and 3) same as F 4) Survey of users receiving shipments; (% of quantity received in kg/yr)
H		1) Survey of shippers; (% of quantity shipped in kg/yr) 2) Expert estimate; (% of quantity shipped in kg/yr)
I	1) U.S. Tariff Commission, P, I, E; (kg/yr) 2) Census of Manufactures; (kg/yr) 3) Minerals Yearbook; (kg/yr) 4) Chemical Economics Handbook; (kg/yr) 5) Chemical Origins and Markets; (kg/yr) 6) NLM/EEC Studies; (kg/yr) 7) NCI Data Bank; (kg/yr) 8) LRPS; (kg/yr) 9) CEH Clipping Files (i.e. trade lit.) 10) "Other" multiclient studies	Same as A
J	Same as I	Same as A
K	NSF EPA (?)	Same as A
L	EPA (?) NIOSH (?)	
M	Numerous sources which provide information on use of chemicals, metals, etc. in products (e.g. CEH, Minerals Yearbook, etc.)	Same as A
N	1) EPA Monitoring Sources 2) Lit. search	

Therefore, Table E-3 reduces the usable release routes and parameters to a more practical level. In effect, the routes of Table E-3 combine the various release routes of Table E-1, and reduce the level of detail and precision to lessen time and cost requirements.

In general, release to the environment resulting from emissions and waste during manufacture will vary widely between companies and even between plant locations within the same company. This was the case with the organic chemicals surveyed for the NSF study. Therefore, on a practical basis, release data for the various phases of manufacture can best be expressed as some percentage of the total production of the chemical or compound.

For the purposes of ranking, it should be possible to determine or estimate the quantities of chemicals released by the routes listed in Table E-3, thus, eliminating many of the gaps that would result from a more complex scheme. Table E-4 gives time/cost estimates.

II Transport, Transformation, and Fate

a. Degradation

The degradation of a chemical in the environment is represented quantitatively in terms of the disappearance of the chemical as a function of time:

$$-\frac{d\ (\text{chemical})}{dt} = k\ (\text{chemical})\ [x]$$

The disappearance is expressed by two types of terms, the rate constant (k) and the concentration(s) [x] of the reactant(s). The rate constant is a measure of the energy of the reaction of the subject chemical with some reacting/attacking species x. The latter may be a chemical oxidant, hydrolytic reagent or microbial agent. The rate constant is independent

Table E-3

RELEASE ROUTES, DATA SOURCES, AND UNITS

Release Route	Data Sources	Units
1) Emissions and waste (EW_R) resulting from manufacturing operations.	1) Emission and waste expressed as a function of production (P). Sources for (P): U.S. Tariff Commission Census of Manufactures Minerals Yearbook CEH Chemical Origins and Markets NLM/EEC Studies NCI NSF Percentage of emission and waste and specific environment (a, w, s, o) to to which released; will be available from: EPA data NIOSH data or by estimate.	1) kg/yr from (P) (x%) where x is an estimate of emission and waste, if quantitative data are not available $EW_R = (P)\ (x\%)$
2) Transportation from producer to point of use. (T_R)	2) Expressed as a function of noncaptive consumption or production. DOT is probably only source. Total release may be negligible by this route.	2) kg/yr from (P) (y%) where y is an estimate $T_R = (P)\ (y\%)$
3) Dispersive use (DU) (any use in which chemical or compound is not chemically changed).	3) Production (P), import (I), and export (E) data. DU = P + I - E - (nonDU) P sources: U.S. Tariff Census of Manufactures Minerals Yearbook CEH Chem. Origins and Markets NCI I, E Sources: U.S. Tariff Dispersive Uses (DU) and (nonDU) Sources: CEH NSF NCI NLM/EEC Chem. Origins and Markets Literature	3) All--kg/yr
4) "Nonintentional" production (release resulting from combustion or use)	4) Monitor sources (EPA, OSHA, and so on) Literature	4) kg/yr

Table E-4

TIME/COST ESTIMATES
(Per Chemical)

Release Route	Information Need	Source	Time (hrs)	Cost (dollars)
1) Emission and waste from manufacturing (EW_R)	1-a) Emission quantities (kg/yr)	1-a) NSF Survey (contains estimates and reported industry values)	(RA)[*] $\frac{1}{4}$	3
	1-b) Waste quantities (kg/yr)	1-b) EPA Data[†]	(RA) 1	12
		1-c) Estimate (as function of production volume and method of manufacture)	(P)[‡] 1	33
		1-d) Survey of manufactures	(P) 2	66
			(RA) $\frac{1}{2}$	6
	1-c) Production (kg/yr) [Emission and waste could be expressed as a function of production (P)]	1-f) U.S. Tariff Commission	(RA) $\frac{1}{2}$	
		1-g) Census of Manufactures	(RA) $\frac{1}{2}$	
		1-h) Minerals Yearbook	(RA) $\frac{1}{2}$	
		1-i) Chemical Economics Handbook	(RA) $\frac{1}{2}$	
		1-j) Chemical Origins and Markets	(RA) $\frac{1}{2}$	66
		1-k) NLM/EEC Studies	(RA) $\frac{1}{2}$	
		1-l) NCI Mark II Data Base	(RA) $\frac{1}{2}$	
		1-m) IARC Monographs	(RA) $\frac{1}{2}$	
		1-n) NSF Study	(RA) $\frac{1}{2}$	
		1-o) Chem. Profiles (ref. CMR)	(RA) $\frac{1}{2}$	
		1-p) CEH clipping files	(RA) 1	
		1-q) Expert estimate	(P) $\frac{1}{2}$	17

---

[*] Research Analyst.

[†] Would require contact with this agency to determine whether emission and waste data are available. Release to various environments (A,W,S,O) should become evident upon review of data.

[‡] Professional.

Table E-4 (Concluded)

Release Route	Information Need	Source	Time (hrs)	Cost (dollars)
2) Transportation from producer to point of use (T_R)	2-a) Reported losses during transport (kg/yr)	2-a) Department of Transportation Annual Report on Hazardous Materials	(RA) ½	6
	OR 2-b) Estimated losses during transport (kg/yr)	2-b) Estimate (by expert) expressed as a function of production. See 1f-1q for sources of production data.	(P) 2	66
3) Dispersive use (DU)	3-a) Situations where chemical is released to the environment as a result of its use. Can be expressed as: DU = (P + I) - [E + (nonDU)] P = U.S. production I = Imports E = Exports NonDU = uses in which chemical undergoes change.	3-a) Published use information on a chemical will generally give both DU (and nonDU) data directly. Such sources are: Chemical Economics Handbook NSF Study NCI Data Bank NLM/EEC Projects Chem. Origins and Markets IARC Monographs CEH clipping files Chem. Profiles (CMR)	(RA) 4 P-2	48 66
		3-b) If it is necessary to determine DU from P, I and E data, the latter are available from: P--(see 1f-1q) I--U.S. Imports (FT-246) E--U.S. Exports (FT-410)	(RA) 6	72
4) "Nonintentional" production (release resulting from chemical or physical processes)	4-a) Reported or estimated production (kg/yr)	4-a) Monitor sources: National Emissions Data System (NEDS) Storage and Retrieval of Aerometric Data (SAROAD) OSHA (?) EPA (?)	(RA) 2	24

Summary: Not all sources would be required for a chemical. Actual cost per chemical would probably range $200-$400.

of concentration but is temperature dependent. The above reaction is referred to as a bimolecular reaction, and is first order in both the chemical and in x. A bimolecular rate constant is given in liter mole^{-1} sec^{-1} or cm^3 molecule^{-1} sec^{-1} (or other appropriate units). The concentration terms (chemical and [x] are expressed in units appropriate to the rate constant, for example, moles liter^{-1}, molecules cm^{-3}, respectively.

In the environment, there are actually many species x_i which may react with a chemical, each having its characteristic rate constant (energy relationship). If we assume only bimolecular processes operating (a simplification for discussion), the rate of disappearance of a chemical is then

$$\frac{-d\ (\text{chemical})}{dt} = \sum_{1}^{n} k_i [x_i][\text{chemical}]$$

$$= [\text{chemical}] \sum_{1}^{u} k_i [x_i]$$

It becomes clear that the major degradation pathways will be those for which the product $k_i[x_i]$ is largest.

An example of the complexity of such potential degradation processes is oxidation in the atmosphere. Laboratory experiments have identified and quantified many different oxygen-derived species which may react with a pollutant. Hydroxyl radical, hydroperoxyl radical, alkoxy radical, ozone, and singlet oxygen are all reactive agents with rate constants ranging from 10^9 to less than 10^{-4} liter mole^{-1}sec^{-1}. Since the rate of the oxidation [-d (chemical)/dt, as differentiated from the rate constant] is dependent also on the concentrations of the reactants, a complete, detailed kinetic expression for atmospheric oxidation is an impossibility. If hydrolysis, microbial degradation, and other fates of the chemical in other environments, are included in the analysis, the large number of unknown factors presents a similar situation.

For chemical degradation, the problem may be approached if data is available on both the rate constant and concentration of the reacting species x for a given process. Calculation of the product $k_i(x_i)$ for a process may then provide some measure of chemical degradation. As a result of the lack of complete data on all reactions (some of which are not measured and some of which may still be unknown), such a number would be a minimal degradation rate. However, the data which are used may represent a dominant degradation process and therefore a more meaningful number. For the consideration of environmental effects, a minimal rate of degradation will at least provide a documentable basis for which to work. Other competitive or more dominant processes would result in more rapid degradation and therefore less of a problem than anticipated.

For the purposes of obtaining a half-life for a chemical in an environmental medium, an assumption or assignment must be made as to a constant concentration of reactant species x. Such an assumption is reasonable if the environment is considered as an infinite sink of such reactants at steady state concentrations (water and oxidants in aquatic environments, ozone, hydroxyl radical, and other oxidants in air). The product $k_i(x_i)$ then represents a new constant value with the chemical still of first order dependence, referred to as a "pseudo-first order reaction." This rate constant is in terms of reciprocal time (min^{-1}, sec^{-1}, etc.). The half-life for a first order reaction is independent of the concentration of a chemical and is given by

$$t_{1/2} = .693/k'$$

Here k' is the product $k_i(x_i)$ and the units of the half-life are defined by the units of the k'. It can be seen that where data are available, the half-life for a chemical undergoing a particular degradation may be evaluated for that process, with the resulting value then representing a maximum half-life in the environment under consideration. Where several processes may be acting simultaneously, the process showing the smallest half-life (greatest rate of reaction for the first order reaction kinetics) is assumed to be dominant, and its half-life is taken as the upper bound of the actual half-life of the subject chemical.

The parameters of degradation in air and water are described more fully in Appendix F. Following are descriptions of other parameters related to the transport and transformation of chemicals in the environment.

b. Vapor Pressure

The vapor pressure for a pure compound at 20°C would be expressed in units of mmHg. If the vapor pressure is not available, knowledge of the boiling point, T_{bp} (at 760 mmHg), allows approximation of the heat of vaporization ΔH_{vap}.

$$\frac{\Delta H_{vap}}{T_{bp}} \approx 21 \text{ cal/deg} \quad \text{(Trouton's Rule)}$$

With the vapor pressure P_1 at another temperature T_1, the value at 20°C may be calculated by

$$\log P_{20^\circ} = \log P_1 + \frac{\Delta H_{vap}}{4.576}\left(1/T_1 - 1/293\right)$$

If necessary, the vapor pressure may be approximated by reference to another compound of similar molecular weight, structure, and boiling point. Vapor pressure citations are given in:

- CRC Handbook of Chemistry and Physics (HCP).
- Langes Handbook of Chemistry.
- J. Timmermans, Physico-Chemical Constants of Pure Organic Compounds, Elsevier, N.Y. 1965.
- T. E. Jordan, Vapor Pressures of Organic Compounds, Interscience, N.Y., 1954.
- Chemical Abstracts, under specific compound or vapor pressure listings.
- Industrial data, manufacturers and suppliers.

c. Partition Coefficients

The partition coefficient is useful in considering the fate of a chemical in water, and also for biological implications. The partition coefficient is a unitless quantity and will be defined as the concentration ratio of the organic solvent to water phase. Partition coefficients in various organic solvent systems are available with direct experimental and some calculated values for octanol/water. The following also may be consulted for semi-quantitative evaluations.

- A. Leo, C. Hansch and D. Elkins, "Partition Coefficients and Their Uses," Chem. Reviews, 71 (6) 1971.
- Chemical Abstracts (under subject chemical and partition coefficients).

d. Occurrence of Chemical in Environment

The occurrence of a chemical in the environment is probably best obtained by EPA from its sources and programs (SAROAD, STORET). As the literature is searched for information on the degradation of the chemical, its occurrence may also be found under various subheadings (for example, analysis of, in soil, water, air, aerosol, and so on). An experienced chemist familiar with the literature would recognize useful information.

e. Biodegradation

Degradation by biological action is probably the dominant process for most chemicals, and especially so in soil and water environments. The rate of degradation of a chemical will be a function of both the specific organisms and the populations, and will vary with the season, climate, and history of the environment (for example, mountain stream, minor and major rivers systems exposed to limited industrial waste disposal, or sewage plant waters). For a useful evaluation of biodegradation of a chemical, we propose a three step effort.

1. A literature search by a person with appropriate training, and an evaluation by a knowledgeable expert. Either extensive studies or simple BOD values available in the literature for some compounds could be used.
2. A BOD experiment using a sewage sample if little or no data is found in the literature. BOD tests are to be determined at 4 inoculate concentrations at times of zero, 15 minutes, and 5 days. Comparison of the differences between the BOD and a sample containing no added chemical would then provide a quantitative measure of biodegradation.
3. If little or no degradation is found in step two, identical BOD measurements would be carried out on an acclimated sewage sample. The need to resort to this experiment would indicate a more recalcitrant chemical.

Biodegradation information can be found in:

Chemical Abstracts, under specific chemical as well as under heading of BOD, Biodegradation, Biological Treatment.

f. More Refined Data Treatments

As the subject chemical is being considered for a STAR, the following paper may be of interest to provide further data:

D. Mackay and A. W. Wolkoff, "Rate of Evaporation of Low Solubility Contaminants from Water Bodies to Atmosphere," Environ. Sci. Tech., 7 (7) 611 (1973).

A half-life may be calculated for loss through evaporation, with the use of available vapor pressures, molecular weights, and solubility data. The calculation requires some reasonable assumptions, such as the water depth and the rates of water evaporation. The calculation may be easily carried out by persons familiar with kinetic calculations.

A second paper approaches the problem of estimating sorption of the chemical onto soil particles.

S. M. Lambert, "Functional Relationship Between Sorption in Soil and Chemical Structure," J. Agr. Food Chem., 15(4) 572.

This paper will be of use if some sorption data on the class of compounds already exists. The parameter used is the parachor, which can be calculated from surface tension, density, and molecular weight data. Parachor can also be calculated from structural parameter considerations. The latter is simpler and reliable, and is suggested for use in this application. When the fate of chemicals absorbed on soil is under consideration, other factors such as humidity, moisture content, soil porosity, and temperature are also important. However, the parachor-soil absorption information will allow at least a semi-quantitative assessment to be made if other soil sorption data are available for comparison and calculation.

g. Time Required

With the use of the references cited, it would require approximately 1/2 day of effort at B.S. level in chemistry to acquire the basic information (solubility, boiling point, vapor pressure, Chemical Abstracts listing, and so on), for each compound. Effort at the Ph.D.-expert level would require a maximum of 2 days per compound; this would include the survey of Chemical Abstracts, literature location, evaluation, and calculations. In many cases a chemical may be completed in less than a day if appropriate information is readily available. It would expedite the evaluations if as many compounds as possible were surveyed in a concerted effort, especially when the same reference sources were being used. The degree of sophistication required to calculate or generate the desired information should be left to the best judgment of the person evaluating the literature. As the data to be obtained are biased toward establishing a minimal degradation rate (maximum half-life), it is necessary that the searcher also recognize any documentable arguments for more rapid degradation that may be generally applicable (direct photolysis, singlet oxygen reactions, catalytic effects in soil, and so on).

The literature search for information on biodegradation would take several hours to locate and evaluate. Depending on the facilities and experience of the contractor (or EPA if done in-house), the BOD measurements would take about 1/2 day per compound. If an acclimated sewage sample BOD run is required, another 1/2 day would be required.

III Toxicology

The toxicological data selected for use in the objective ranking system for chemicals were chosen on the basis of estimated availability and utility. Emphasis was placed on data resulting from controlled experimentation with laboratory animals rather than on data derived from field observations--including epidemiological and human case history investigations--because data from controlled experimentation more closely meet our selection criteria.

The types of data we have selected include threshold limit values for workroom spaces, LD50 values, and minimum dosages demonstrated to produce chronic toxicological effects--including carcinogenic, mutagenic, and teratogenic effects. Except for acute toxicity in aquatic organisms, there is little information published on the toxicity of chemicals to nonmammalian animals. In acute toxicity tests with aquatic organisms, the LC50 values derived from survival data are often based on different exposure times and thus are difficult to equate. For this reason, we have not included nonmammalian toxicity data.

The most likely ways that man may be poisoned by an environmental chemical are by ingestion, contact with the skin, or inhalation; consequently, we recommend the use of data obtained in studies in which the oral, dermal, or pulmonary route of exposure was used. We also recommend that for all in vivo studies the administered amounts be converted to mg/Kg units. Exposure concentrations administered in inhalation studies should be converted to weight units. Admittedly, this conversion is subject to error. Average respiratory rates and tidal volumes required for this conversion are presented for various animals in the Biology Data Book (FASEB, 1964).

a. Threshold Limit Values

Threshold limit values (TLV) for workroom spaces have been established by OSHA to minimize exposure hazard to workers. TLV's have also been assembled for many chemicals by the ACGIH. The values are based on animal and human toxicological data and are expressed in parts per million (ppm) or mg/m^3. The list of values published by OSHA or ACGIH represent 8-hour weighted averages or ceiling values that are well-defined.

We recommend rating those chemicals for which TLV's are available in the following manner:

Rating	TLV (ppm)
1	> 1000
2	500-1000
3	100- 500
4	50- 100
5	10- 50
6	< 1

b. Acute Toxicity

Acute toxicity tests are usually the first type of test performed on a chemical of unknown toxicity. Such tests are usually intended to provide survival data from which the dose or concentration that will kill 50% of a test population may be estimated. This dose is called LD50. A rating system that may be used for LD50 values follows:

Rating	LD50 (mg/Kg)
1	> 5000
2	500-5000
3	50-5000
4	1- 50
5	< 1

In that the toxicity of a compound often varies with the route of administration, species of test animal, age, physiological state, and other factors, we recommend that use be made of average LD50 values. If no toxicity data are available for a chemical, we recommend, as a minimum, that the LD50 (oral) be obtained experimentally using either the rat or mouse. Such a test will cost less than $1000.

Sources of LD50 values, in the suggested search sequence, are the Toxic Substance List, Handbook of Toxicology (Spector), TOXLINE/MEDLINE/CBAC, the Merck Index, Farm Chemicals Handbook (pesticides only), Biological Abstracts, Index Medicus, and Chemical Abstracts.

c. Repeated Dose Effects

Repeated dose toxicity studies are usually designed to determine the effects of long-term exposure to sublethal doses of a chemical. The duration of exposure may be up to 90 days (subchronic toxicity test) or may extend throughout the normal life span of the test animal (chronic toxicity test). During the course of a repeated dose study, many different observations may be made. These observations include body weight, behavior, organ function, gross and histopathology, hematology, physiology, biochemistry, metabolism, life span and others.

Some of the observed effects may have less significance in terms of the well-being of the organism than others; hence, the operator of the ranking system should attempt to categorize the reported effects in order of increasing biological significance. An experienced toxicologist may be needed for this task. Categories that may be used are listed below.

Rating	Category
1	Chemical accumulates in tissues without apparent effect.
2	Chemical produces effects of uncertain biological significance.
3	Chemical produces effects related to disease.
4	Chemical produces a persistent disease state.
5	Chemical significantly reduces the life span of the organism.

Chemicals in each category should then be ranked according to the minimum dose that produces an effect of significantly greater magnitude or frequency than observed in the controls. By studying the data collected, the operator of the ranking system should be able to devise a rating system similar to that suggested for ranking LD50 values.

Although there are numerous reports on subchronic and chronic toxicity of chemical substances, there is no single comprehensive source. The Toxic Substances List may be used as a guide in determining if a chemical has been subjected to subchronic or chronic exposure evaluation;

however, information provided in this document is limited. A search of computerized data banks such as TOXLINE, MEDLINE, and CBAC should not be omitted, as they provide ready access to the more recent literature. By and large, the most useful sources are Biological Abstracts, Index Medicus, and Chemical Abstracts. Searching these sources is usually very time-consuming; however, the task can be greatly expedited by photocopying pertinent sections of the cumulative indices, flagging the abstracts, and, via computer, organizing the abstract numbers in ascending order according to volume and journal for all chemicals of interest. Using the resulting list, a relatively untrained person should be able to photocopy the abstracts quickly and efficiently. The photocopied abstracts should then be reviewed by the data extractor. Original articles should be retrieved only if, for a given study, information required by the objective ranking system is not given in the abstract.

d. Carcinogenicity, Mutagenicity, and Teratogenicity

Chemicals for which carcinogenic, mutagenic, or teratogenic action have been demonstrated should be placed at or near the top of a list of chemicals ranked in terms of toxicity, regardless of other toxicological information that may have been collected. If it becomes necessary to rank those chemicals that produce any one of these effects in terms of relative potency, the operator of the overall ranking system may devise a rating system based on dose.

A major source of information on chemical carcinogens is PHS-149, a listing of chemicals that have been tested. Information may also be obtained by contacting the National Cancer Institute. A limited amount of information can be found in the Toxic Substances List. The Environmental Mutagen Information Center (EMIC) maintains a fairly up-to-date list of citations pertaining to chemical mutagenesis and is probably the best single source of information on mutagens. The Center does not abstract the original article; hence, to obtain specific information, the full-text document must be retrieved. Teratological information may be found in the Catalog of Teratogenic Agents (Sheppard), and up-to-date information may be obtained by consulting "Teratology Lookout," a monthly newsletter of the Karolinska Institute.

e. Time Required

Personnel

Literature Specialist: Experienced in searching computerized data bases, Chemical Abstracts, Biological Abstracts, and Index Medicus. Should be knowledgeable on journal inventory of nearby libraries.

Biologist, B.S. or M.A.: Physiology and/or toxicology background.

Toxicologist, Ph.D.: Working experience in mammalian toxicology.

Duties

- The major responsibilities of the literature specialist are:

  Conduct searches of computerized data bases.

  Search indices of the various abstract journals and organize abstract numbers.

  Retrieve pertinent abstracts selected by the biologist.

- The responsibilities of the biologist are:

  Extract, organize, and prepare data for use in the ranking system. Assist literature specialist in data search (i.e., supply supervision as needed).

- The toxicologist is responsible for the overall supervision of the task as well as for devising suitable rating systems for the various toxicological parameters.

Time Involvement (per chemical basis)

Literature specialist: 12-15 hours

Biologist: 16-20 hours.

Toxicologist: 3-5 hours.

IV Modifications for Mathematical Model

In the recommended lists of parameters, only a few changes were made to fit the abilities of the objective procedure to model an agent's behavior in the environment.

In the area of release, we eliminated data on other (O) disposal, for instance to deep wells, as being too infrequently available for use and too difficult to model.

In the area of fate, we could not find an easy way to express the effect of the partition coefficient in determining the retention of agents in biological systems. However, the information could be used in ad hoc studies. In addition, we found it necessary to add essentially non-parametric data on transport and dilution as a component of this area.

In the area of toxicology, the model system requires a more definitive relationship between probable exposures and likely incidences of effects than are provided by the simple numerical ranking system suggested. The difficulties in translating biological data into predictive models are well known. However, for the purposes of priority ranking, the uncertainties are less important, because any information is more useful than no information at all. Accordingly, the systematic procedure in Appendix F recommends that the parameters suggested in the toxicology section be translated into dose-response curves by as crude methods as are justified.

Appendix F

PROCEDURES FOR OBJECTIVE RANKING

Appendix F

PROCEDURES FOR OBJECTIVE RANKING

The objective subsystem defines procedures for acquiring information about the agent under consideration, processing that information, and using the results to rank the agent with respect to other agents already ranked. We take the position that these procedures should be as explicit as possible for the most commonly expected types of agents. However, the system cannot be designed to cope with all possible types of agents; in fact, it would not be cost effective to provide complete procedures for agents that will rarely be encountered as STAR candidates.

Examination of the lists of agents currently proposed for STARs and of those for future consideration reveals that most exert their effects through chemical action on biological systems. These effects include known and suspected effects on human health and on nonhuman fauna and flora. Some (for example, PCBs) are suspected of having more subtle ecosystem effects, while others have additional effects on the nonliving environment (for example, sulfates, if sulfuric acid is included). Therefore the objective subsystem is designed with a main thread that includes characterization of the agent chemically; examination of its occurrence in the environment from natural and manmade sources; prediction of its environmental transport, transformation, and fate; estimation of its toxic effects; and valuation of those effects. Less attention is given to the effects of chemicals on the nonliving environment, the biological effects of nonchemical agents, and other even less frequently encountered effects.

The system for objective ranking consists of a set of procedures called branches that are labelled A through Z. Each procedure consists

Preceding page blank

of a series of steps. Each step is either a state-of-information test or an information processing step, as shown in Figure F-1, and is structured as follows:

Step Number	Test or Processing Instructions	Next Step Number

(In the case of state-of-information tests, the next step depends on the answer to the test.) To avoid repetitive questions some tests have multiple answers.

When an agent gives a positive response to the state-of-information tests, it is processed through BRANCH A, the main branch of the system, which gathers and processes information about the environmental release, fate, and biological effects of chemicals. Negative responses take the operator into other branches of the system, but when the proper information has been gathered and processed, he returns to some point further down the main branch.

Some steps of BRANCH A direct the operator to other branches, which each start on a new page. The direction to the "next step" consists of a branch index (A,B,. . .Z, AA, . . .) and a step number. Major branches often have further minor branches, but the flow is always eventually directed back to BRANCH A.

Two special symbols are used to indicate further instructions. The * indicates that the system operators must exert more than minimal subjective judgement in answering tests or processing information. The frequency of *'s in the procedure demonstrates that the subsystem has substantial subjective inputs and is thus only "more objective" than the expert system, in that explicit decisions are made. The † indicates that additional information for answering the test or processing the information

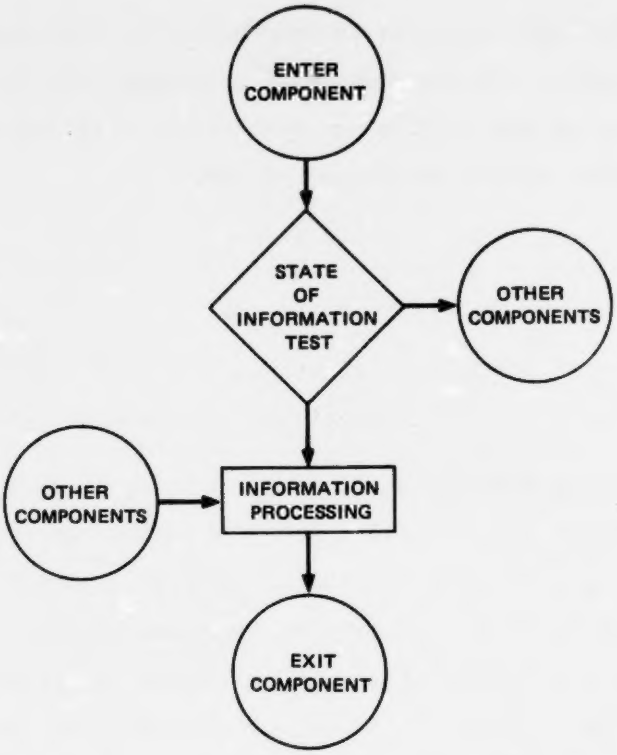

ENTER COMPONENT
STATE OF INFORMATION TEST
OTHER COMPONENTS
OTHER COMPONENTS
INFORMATION PROCESSING
EXIT COMPONENT

FIGURE F-1 GENERALIZED SYSTEM FLOW COMPONENT

is given on additional pages labeled with the step number. For example, work sheets to be completed are so indicated.

Economy must be kept clearly in mind in carrying out the procedure. The first information found should be accepted as definitive, unless it is clearly suspect. Complex branches should not be entered unless the need is clear. The procedure is designed to get only a better ranking of priorities, not a perfect one.

In the same spirit, an attempt should be made to go through the entire procedure and identify all of the questions that are not readily answered. Some of the answers that are available may suggest that some of the questions need not be answered. For example, if half-lives in water are exceedingly short, it is unnecessary to look hard for aquatic toxicological data. All the unanswered questions (the Z1s) should be collected before ad hoc studies are authorized. The combined cost of all ad hoc studies should not exceed $3,000.

Note: There are no Branches N, O, P, R, T, U, W, X, or Y at present.

Ranking Procedure

BRANCH A--MAIN FLOW

Step Number	Start		Next Step Number
A1	Start with a trace of the procedure worksheet.† Is the agent well defined?	Yes*	A2
		No	B1
A2	Prepare agent identification sheet† and proceed to		A3
A3	Is the potential for environmental harm reasonably clear?	Yes*	A4
		No	B3
A4	Complete preliminary effects checklist,† acquire basic documents* (criteria documents, legislative/regulatory history, reviews, data sheets). Continue to		A5
A5	Does the agent exert its environmental effects through its chemical properties?	Yes	A6
		No	C1
A6	Is it a compound or well defined mixture?	Yes	A7
		No	D1
A7	Retrieve CAS number if not already known. Use CHEMLINE, TSL, TMIC, CAS, proceed to		A8
A8	Is the chemical organic?		A9
	elemental?		G1
	metallo-organic?		H1
	other inorganic?		I1
A9	Look for production information in (1) SOC; (2) NSF; (3) Census; (4) CEH; (5) NCI.		A9
A10	Production information found?	Yes	A11
		No	AA1

BRANCH A--Continued

Step Number			Next Step Number
A11	Look for import and export information in (1) FT-246+FT-410; (2) NSF; (3) CEH		A12
A12	Import and export information found?	Yes	A13
		No	AB1
A13	Look for intermediate and dispersive use information in (1) NSF; (2) CEH; (3) NCI; (4) COM		A14
A14	Intermediate use information found?	Yes	A15
		No	AC1
A15	Express information in kg/yr. Compute dispersive use, (DU), by $DU = P + I - E - IU$, where P = production, I = imports, E = exports, and IU = intermediate usage. Check with DU information from step A13, and adjust as appropriate.*		A16
A16	Look for information on fraction of production to air emissions, water effluent, and land disposal of solid waste in (1) NSF; (2) EPA reports; (3) NIOSH reports; (4) other basic documents		A17
A17	Adequate information found?	Yes	A18
		No	AD1
A18	Look for information on fraction of dispersive use to air, water, and land in (1) NCI; (2) NSF; (3) WPPMP; (4) basic documents		A19
A19	Adequate information found	Yes	A20
		No	AE1

BRANCH A--Continued

Step Number | **Next Step Number**

A20 Express information from steps A16-A19 either directly as discharges to air, water. and land or in terms of e_A (fractional emissions to air), e_W (fractional emissions to water), e_L (fractional emissions to land), f_A (fraction of dispersive use to air), f_W (fraction of dispersive use to water), and f_I (fraction of dispersive use to land). In the latter case, compute releases to air, water, and land by multiplying the e's by P and the f's by DU. Complete release work sheet.† A21

A21 Is there occasion to believe transportation losses might be significant?
Yes. AF1
No A22

A22 Examine the information on production location, dispersive uses, transportation, and other releases to the environment.† Is there reason to believe that the releases are concentrated in localized areas?
Yes. AG1
No A23

A23 Look for information on air oxidation rate constants in (1) Wilson; (2) ACS; (3) Doyle; (4) CA. A24

A24 Rate information satisfactory?
Yes. A25
No J1

A25 Compute air half-life T_A by†

$$T_A = \frac{0.693}{10^{-15}k_{OH} + 2 \times 10^{-9}k_{O_3}}$$

where k_{OH} and k_{O_3} are the rate constants, in $(Yr)^{-1}$/Mole for hydroxyl and ozone oxidation. A26

BRANCH A--Continued

Step Number			Next Step Number
A26	Look for information on oxidation in aqueous systems or hydrolysis in (1) Hendry; (2) CA		A27
A27	Rate information satisfactory?	Yes	A28
		No	J1
A28	Compute water half-life T_W by † $$T_W = \frac{0.693}{10^{-10}k_{RO_2} + k_h}$$ where k_{RO_2} is the rate constant, in $(Yr)^{-1}$/mole fraction, for alkylperoxy radical oxidation and k_h is the pseudo first order rate constant for hydrolysis at pH ~ 7.		A29
A29	Look for parachor information in Lambert.		A30
A30	Rate information satisfactory?*	Yes	A31
		No	J1
A31	Compute land half-life T_L from rate information.† Is biodegradation likely?	Yes	Q1
		No	A32
A32	Compute steady-state inventories, SSI, of the chemical in the media from equations of the form $$SSI_A = R_A T_A/0.693,$$ where R_A is (for example) the total release per year to air†.		A33

BRANCH A--Continued

Step Number			Next Step Number
A33	Examine the available information to determine[*] whether significant departure from steady-state conditions are likely. Look particularly at (1) rapid growth or curtailment of releases in past 10 years, (2) half-lives greater than 10 years, (3) suggestion that disappearance is not clearly related to amount present..		A34
A34	Adjustments indicated?	Yes	K1
		No	A35
A35	Examine the available information to determine[*] whether intermedia transfers are likely to be significant. Look particularly for (1) volatility (water + land → air) or lack of it, (2) water solubility (air + land → water) or lack of it, (3) affinity for sorption on particulate material (air + water → land), or lack of it.		A36
A36	Adjustments indicated?	Yes	L1
		No	A37
A37	Examine dispersive uses, other production sites, methods of disposal, physical/chemical parameters, and so on, to determine[*] whether any populations (not all human, but other animate and inanimate) are likely to be uniquely exposed.[†]		A38
A38	Special populations?	Yes	M1
		No	A39
A39	Separate the steady-state inventories of the agent in the various media by the dilution factors shown on the transport work sheet (A32).[†] Calculate corresponding concentrations.		A40
A40	Are there any biological effects?	Yes	A41
		No	S1

BRANCH A--Concluded

Step Number		Next Step Number
A41	Prepare a biological effects checklist.† Select* no more than five species at risk. For man, select* no more than three dominant effects; for other species, no more than one.	A42
A42	Effects related to a "dose" to species.	
	Yes	A43
	No	E1
A43	Look for dose-response relationships in (1) basic documents; (2) limited search of literature, e.g., TOXLINE	A44
A44	Any data? Yes	A45
	No	F1
A45	Express* information in terms of a graph of incidence of effect (probability/yr) versus dose (kg/yr or other natural units). Integrate† incidence by distribution of dose over population of targets (human, biological, and other). For example, if the same dose applies to all members of a population N, and the corresponding incidence is I, then the expected number of cases is NI. Repeat for each effect..	A46
A46	Effects valued in accompanying table?†	
	Yes	A47
	No	V1
A47	Multiply cases by values to obtain ranking index for effects. Add indexes for all effects to obtain the environmental hazard index for the chemical.†	A48
A48	Compare environmental hazard index to those of agents already ranked. Insert agent in list at appropriate rank order, and reorder ranks of lower-ranking agents.	END

BRANCH AA--NO PRODUCTION INFORMATION

Enter from A10, I2

Step Number	Start	Next Step Number
AA1	Is the chemical known to be produced as part of a class whose production is known? Yes	AA2
	No	AA3
AA2	Divide production of class by number of chemicals in class. Adjust* upward or downward if chemical is known to be a major or minor contributor, respectively	A11 or I3
AA3	Is the chemical known to be in commercial production? Yes	AA4
	No	AA5
AA4	Set production provisionally at 10,000 kg/yr. Reject this figure if dispersive use information later overweighs it	A11 or I3
AA5	Are the significant sources of the chemical anthropogenic, even though unintentional? Yes	AA6
	No	AA9
AA6	Estimate* release to environmental media from known sources, from basic documents	AA7
AA7	Any problems? Yes	Z1
	No	AA8
AA8	Complete release worksheet A20	A22
AA9	Are there controllable human activities which influence the movement and distribution of the chemical in the environment? Yes	AA10
	No	B4

BRANCH AA--Concluded

Step Number		Next Step Number
A410	Estimate* contribution of human activities to excess inputs to the environmental media from basic documents.	AA11
AA11	Any problems? Yes.	Z1
	No	AA12
AA12	Complete release worksheet A20.	A22

BRANCH AB--NO IMPORT/EXPORT[1] INFORMATION

Enter from A12, I3

Step Number	Start		Next Step Number
AB1	Any suggestion* that imports/exports are significant?		
		Yes.	AB2
		No	AB5
AB2	Estimate* imports/exports		AB3
AB3	Any problems?	Yes.	Z1
		No	AB4
AB4	Go to		A13 I4
AB5	Imports/exports = 0		A13 I4

---

[1] Complete for imports only, exports only, or both as appropriate.

BRANCH AC--INTERMEDIATES

Enter from A14, I4

Start

Step Number		Next Step Number
AC1	Is the intermediate use suspected* to be:	
	Major	AC2
	Minor	AC3
	Negligible	AC4
	Unknown	AC5
AC2	IU = 0.9(P + I - E)	A15 I5
AC3	IU = 0.3(P + I - E)	A15 I5
AC4	IU = 0.	A15 I5
AC5	IU = 0.5(P + I - E)	A15 I5

BRANCH AD--PRODUCTION LOSSES[1]

Enter from A17

Start

Step Number			Next Step Number
AD1	Is the chemical a gas or relatively volatile (vapor pressure > 80 mm Hg)?	Yes	AD4
		No	AD2
AD2	Is there information to suggest the chemical is released to the air as a particulate?	Yes	AD4
		No	AD3
AD3	$e_A = 0$		AD6
AD4	$e_A = 0.05$		AD5
AD5	Examine basic documents and adjust* e_A downward if justified.		AD6
AD6	Is the chemical produced in a process that has a significant chance of water discharges?	Yes	AD7
		No	AD9
AD7	$e_W = 0.05$		AD8
AD8	Examine basic documents and adjust* e_W downward if justified.		AD10
AD9	$e_W = 0$		AD10
AD10	$e_L = 0.05$		AD11
AD11	Examine basic documents and adjust* e_L downward if justified.		AD18

---

[1] Use the default values from this sheet only for those media with inadequate information.

BRANCH AE--DISPERSIVE RELEASE[1]

Enter from A19

Start

Step Number			Next Step Number
AE1	Estimate* fraction f_r that accumulates in a relatively inaccessible reservoir (e.g., dyes in glass products)		AE2
AE2	Is the chemical a gas or quite volatile (vapor pressure > 120 mm Hg)?	Yes	AE3
		No	AE4
AE3	$f_A = 1 - f_r$		AE7
AE4	Is it somewhat volatile (vapor pressure > 40 mm Hg)?	Yes	AE5
		No	AE6
AE5	$f_A = 0.3\ (1 - f_r)$		AE7
AE6	$f_A = 0$		AE7
AE7	Is it known to be disposed of in water (e.g., an ingredient of soaps and detergents)?	Yes	AE8
		No	AE9
AE8	$f_W = 1 - f_r - f_A$		AE12
AE9	Is it known not to be disposed of in water?	Yes	AE10
		No	AE11
AE10	$f_W = 0$		AE12
AE11	$f_W = 0.5\ (1 - f_r - f_A)$		AE12
AE12	$f_L = 1 - f_r - f_A - f_W$		A20

---

[1] Use the default values from this sheet only for those media with inadequate information.

BRANCH AF--TRANSPORTATION LOSSES

Enter from A21

Start

Step Number		Next Step Number
AF1	Obtain information from TADS in EPA and from the DOT Office of Hazardous Materials, if available. Express the losses in kg/yr, average, to air, water, and land. Enter information on Worksheet A22. Add to releases calculated in A20	AF2
AF2	Any problems? Yes	Z1
	No	AF3
AF3	Return to	A22

BRANCH AG--LOCALIZED RELEASES

Enter from A22

Step Number	Start		Next Step Number
AG1	Examine information on localization with particular attention to release into closed systems (e.g., homes, holding ponds, dumps), in short, any system that would sharply limit the dispersal into the general environment. Develop a description of these limited environments that includes (1) media involved and quantities (m^3 air, l water, m^2 land); (2) populations of targets (human, other living and nonliving) in the local environment; (3) routes of escape to the general environment. Enter data on Worksheet A22. Save information for Step A39.		AG2
AG2	Any problems?	Yes	Z1
		No	AG3
AG3	Return to		A23

BRANCH B--EARLY CLARIFICATION

Enter from A1

Start

Step Number			Next Step Number
B1	Request further definition and identification from nominator.		B2
B2	Was clarification satisfactory?	Yes	A2
		No	B3

Enter Also from A3

Step Number			Next Step Number
B3	Request identification from nominator.		B4
B4	Is the nature of the agent and its potential hazard now clear?	Yes	A4
		No	END

BRANCH C--NONCHEMICAL AGENTS

Enter from A5

Step Number	Start	Next Step Number
C1	Determine whether the agent's action is Radiological. . . . . Physical. . . . . Biological. . . . . Other.	 CA1 CB1 CC1 C2
C	Reexamine agent definition and justification for consideration.	C3
C3	Same conclusions? Yes. . . . . No	 C4 C1
C4	Check Worksheet A2 carefully. Prepare materials on the ranking procedure, with several diverse examples. Identify expert in area, inside or outside EPA. Request ad hoc ranking relative to several indicator agents. Budget #3,000 or less. Return to	A48

BRANCH CA--RADIOLOGICAL AGENTS

Enter from C1

Step Number	Start		Next Step Number
CA1	Define the limits of the agent carefully. For example, is the radiation associated with a particular radionuclide? Is it ultraviolet radiation, but only that associated with decreases in the ozone shield? If microwave radiation, what are the frequency limits?		CA2
CA2	Is the radiation ionizing?	Yes No	CA3 CAA1
CA3	Describe the radiations, the mode of their release, and the targets in the environment		CA4
CA4	Can dose distributions, in terms of rads or rems to organs or the whole body, be described easily from basic document data	Yes No	CA5 CAB1
CA5	Determine the at-risk populations and doses (rad/yr) they face. Assume linear dose-response relationships with slopes as given in Table.[†] Compute incidences of effects and integrate		CA6
CA6	Effects valued in Table A46?	Yes No	CA7 V1
CA7	Multiply cases by values to obtain ranking index for effect. Repeat for other effects. Add indexes for all effects to obtain the environmental hazard index for the agent. Return at.		A48

BRANCH CAA--NONIONIZING RADIATION

Enter from CA2

Step Number	Start		Next Step Number
CAA1	Determine whether radiation is (1) ultraviolet; (2) visible; (3) infrared; or (4) other. Obtain relevant literature, which should be rather limited. Attempt to quantify field intensities (joules/m^2), durations (e.g., hours per year), and exposed population.		
CAA2	Any problems?	Yes.	Z1
		No	CAA3
CAA3	Determine effects due to intensity distributions as estimated. For example, there is a 50% probability of blindness associated with Z joules/m^2 of ruby laser light if delivered in under 1 second. Integrate incidence by distribution of dose over population of targets. Use basic documents and collected literature		CAA4
CAA4	Any problems?	Yes.	Z1
		No	CAA5
CAA5	Effects valued in Table A46?	Yes.	CAA6
		No	V1
CAA6	Multiply cases by values to obtain ranking index for effects. Repeat for other effects and add indexes for all effects to obtain the environmental hazard index for the agent. Return to.		A48

BRANCH CAB--RADIATION DOSE DISTRIBUTION

Enter from CA4

Step Number	Start	Next Step Number
CAB1	Determine whether the radiation is	
	Alpha.	CABA1
	Beta.	CABB1
	X or gamma.	CABC1
	Other.	CAB2
	A combination.	CAB4
CAB2	Define the release and distribution of the radiation and/or its carrier as well as possible from basic documents.	CAB3
CAB3	Can dose distributions be estimated?*	
	Yes.	CA5
	No	Z1
CAB4	Repeat from Step CAB1 for each radiation involved	CA5

BRANCH CABA--ALPHA RADIATION

Enter from CAB1

Step Number

Start

Next Step Number

CABA1 Determine release and distribution of carrier (for example, radon) in environment as for chemicals. Determine radioactive half-life (T_R, yr) and energy (E, Mev) of decay. Set relative biological effectiveness (RBE) to 10. Estimate annual atoms of intake for exposed populations, using exposure factors in Table A45.1. Determine biological half-life, T_B, if available from basic documents or Miller. If not available assume it is 50 years. Compute net half-life (T_N) as

$$\frac{1}{T_N} = \frac{1}{T_R} + \frac{1}{T_B}$$

CABA2 Estimate body burden (B) of carrier as

$$B = R \frac{T_N}{0.693}$$

and annual disintegrations (R'), as

$$R' = 0.693 \frac{B}{T_R} = R \frac{T_N}{T_R}$$

where R is the annual rate of intake. Estimate the annual effective dose as

$$1.6 \times 10^{-8} \frac{\text{rad}}{(\text{Mev/g})} (\text{RBE}) \frac{R'E}{m}$$

where m is the mass (g) of the organ of concentration.† Use the whole body if not known. Return to. CA5

BRANCH CABB--BETA RADIATION

Enter from CAB1

Step Number		Next Step Number
	Start	
CABB1	Determine whether radiation is associated with a carrier (e.g., tritium) or with some other source of electrons (e.g., accelerators). If the latter, devise ad hoc procedure for estimating dose distribution from basic documents or go to Z1. Otherwise, determine release and distribution of carrier in environment as for chemicals. Determine half-life (T_R, yr) and average energy (E, Mev) of decay. Set RBE to 1. Estimate annual atoms of intake for exposed populations, using exposure factors in Table A45.1. Determine biological half-life, T_B, available from basic documents or Miller. If not available, assume it is 50 years. Compute net half-life T_N as $$\frac{1}{T_N} = \frac{1}{T_R} + \frac{1}{T_B}$$ Continue as in	CABA2

BRANCH CABC--X AND GAMMA RADIATION

Enter from CAB1

Start

Step Number		Next Step Number
CABC1	Determine whether radiation is associated with	
	A carrier (e.g., Cesium 137)	CABC2
	Other source of photons	CABC4
CABC2	Determine--on the basis of modes of release and exposure, affinity for body organs, and so on--whether the carrier is likely to be significant as a source of radiation	
	Externally to the body	CABC4
	Internally	CABC3
CABC3	Set RBE equal to the fraction of dose remaining in the organ (from Miller)	CABB1
CABC4	Devise ad hoc procedure for estimating dose distribution from basic documents	CABC5
CABC5	Successful? Yes	CABC6
	No	Z1
CABC6	Return to	CA5

BRANCH CB--PHYSICAL AGENTS

Enter from C1

Step Number	Start	Next Step Number
CB1	Quantify agent's discharge to environmental media. For example, if the agent is waste heat, quantify the energy flow (cal/yr) into air and water. If it is particulate matter or solid waste, quantify the kg/yr to air, water, and land. Use units appropriate* to effects of concern. Use basic documents where possible. If results unsatisfactory,* do limited literature search, or as a last resort, contact knowledgeable people in government and industry	CB2
CB2	Estimate the environmental half-life (T_E, yr) in the media of concern. Use any information in the basic documents, computation, limited literature survey, or (as a last resort), expert opinion	CB3
CB3	Estimate dilution or dissipation factor(s) appropriate to various media and populations affected. For example, particulates should be assumed diluted in air over a volume bounded by the aggregate areas of metropolitan regions affected and the height of the mixing layer, say 100-200 meters. Use basic documents to determine regions affected. Units as appropriate, e.g. (liters)$^{-1}$ for water. See also Tables in A39.	CB4
CB4	Any Problems? Yes. . . . . No	Z1 CB5
CB5	Estimate the steady state concentration, C_s, in the media by $C_s = RD\ T_E/0.693$, where R is the release rate in kg/yr, D is the dilution factor, and T_E is the half-life. Adjust as appropriate* if steady-state unlikely (R not constant, T_E very long, and so on).	CB6

BRANCH CB--Concluded

Step Number		Next Step Number
CB6	Are effects related to a "dose" to target?[1]	
	Yes.	CB7
	No	E1
CB7	Dose-effect relationship known? Yes.	CB8
	No	F1
CB8	Express information in terms of a graph of incidence of effect (probability/yr) versus dose (kg/yr or other natural units). Integrate (A45) incidence by distribution of dose over populations of targets. For example, if the same dose applies to all members of a population N, and the corresponding incidence is I, then the expected number of cases is NI. Use basic documents, or other known source of such information	CB9
CB9	Are effects valued in Table A46? Yes.	CB10
	No	V1
CB10	Multiply cases by values to obtain ranking index for effect. Repeat for other effects. Add indexes for all effects to obtain the environmental hazard index for the agent. Return to.	A48

---

[1] Relate dose to concentration through exposure factors in various media for targets. For example, human water intake 500 l/yr, and dose = $C_{water} * 500$. See exposure factors in Table A45.1, or estimate from very limited literature search. Little information generally available.

BRANCH CC--BIOLOGICAL AGENTS

Enter from C1

Start

Step Number		Next Step Number
CC1	Develop* an ad hoc procedure,[1] within budget limit of $3,000, that would incorporate some of the following ideas: Division by class: viral, bacterial, rickettsial, protozoan, higher forms Reference to monitored values of concentration, e.g., from STORET for coliform in water Consideration of vectors for transmission Valuation on basis of disease potential	. . . . .A48

---

[1] Enough is known about biological agents that this branch could be developed to the detail of Branch CA for a few hundred dollars. However, with the possible exception of viruses in drinking water, EPA has little jurisdiction over such problems and the likelihood of a STAR nomination is low.

BRANCH D--CHEMICAL DEFINITION

Enter from A6

Start

Step Number		Next Step Number
D1	Determine whether the agent is	
	a mixture of isomers (e.g., cresols) or of similar compounds (e.g., long chain fatty acids).	DA1
	an element[1] and its important compounds (e.g., mercury), or all compounds with a similar functional group (e.g., sulfates or cyanides), or a group of chemicals with similar uses (e.g., oil dispersants)	D2
	a natural product	DB1
	other	D2
D2	Define chemicals included in group	D3
D3	Is the group sufficiently* homogeneous that one member can be chosen as representative Yes.	D4
	No	D5
D4	Choose* representative	A7
D5	Complete Worksheet D5.† For each important member of the group, complete Worksheets A2 and A4. Then go successively to A7-A47; add environmental hazard indices for all chemicals to obtain index for groups. Return at	A48

---

[1] See also Branch G.

BRANCH DA--HOMOGENEOUS MIXTURES

Enter from D1

Start

Step Number			Next Step Number
DA1	Are there any significant* differences among compounds in the mixture?	Yes	DA2
		No	D4
DA2	Define several representatives		D5

BRANCH DB--NATURAL PRODUCTS

Enter from D1

Step Number	Start		Next Step Number
DB1	Search for information on composition of product in Merck, CTCP, primary literature.		DB2
DB2	Any problems?	Yes	DB3
		No	D5
DB3	Attempt to continue from A7 using agent as a defined but not chemically characterized mixture		A7

BRANCH E--EFFECTS UNRELATED TO DOSE

Enter from A42, CB6

Start

Step Number			Next Step Number
E1	Reexamine definitions to see if a dose-effects relationship could be constructed.		E2
E2	Same conclusions?	Yes	E3
		No	E5
E3	Define effects through known concentrations in media and descriptions of targets and responses in basic documents.		E4
E4	Any problems?	Yes	Z1
		No	E5
E5	Return to next step		A43 CB7

BRANCH F--DOSE/EFFECTS

Enter from A44, CB7, SA3

Start

Step Number		Next Step Number
F1	Dose-effect relationships are generally rather difficult and expensive to develop unless quite a bit of information is available. Devote a very limited time to searching the literature for such information. Otherwise, assume a linear relationship with no threshold unless empirical or a priori information suggests otherwise. The only parameter needed then is the slope. This can be determined by estimating the dose at any specified incidence, e.g., LD50. The estimate will be more conservative as the specified incidence approaches 1.0. Use 1.0 incidence if the dose exceeds that for 1.0 incidence.	F2
F2	Return to next step	A45 CB8 SA4

BRANCH G--ELEMENTS

Enter from A8

Step Number		Next Step Number
Start
G1	This branch applies to elements like mercury or selenium. In most cases, the description of agents that go by the name of elements actually imply elements and their compounds (see D1). When possible, it is best to separate each compound out and run it through the appropriate branch (e.g., branch H for methylmercury, Branch I for mercuric or mercurous species). There is then no need to discriminate between the elemental form and inorganic compounds.	G2
G2	Separation made?
(metallo-organic) Yes.	H1
(inorganic) Yes.	I1
No	G3
G3	If it is infeasible to separate individual compounds for ranking, consider the element as an entity in all of its forms. Clearly, the element is neither created nor degraded, and the total amount is fixed (disregarding radioactive transformation). What is important, is only the redistribution by man. This can be estimated* from MY (for production, imports, and exports), CEH (for dispersive uses), and the basic literature--especially NAS monographs and NSF trace contaminants studies. Census and NCI may also be useful in this regard. Fractions to various media from extraction, processing, chemical conversions, and use can sometimes be estimated from emissions factors for trace substances and the above sources.	G4
G4	Any problems?
Yes.	G5
No	G7

BRANCH G--Concluded

Step Number		Next Step Number
G5	Attempt to go through main organic chemical branch Steps A10, A12, A13, A15, A17, A19, And A20, branching to the default values where necessary; then return to.	G6
G6	Any problems? Yes. No	Z1 G7
G7	Perform Steps A21 and A22.	G8
G8	Estimate,* from basic documents and limited literature search, the half-lives in air, water, and land for the element. The removal processes are transfers to relatively inaccessible reservoirs like binding to sediments or soils, or burial in impermeable landfills.	G9
G9	Perform Steps A32-A40.	G10
G10	Complete a biological effects checklist (A41). For agents specified only to the elemental level, it will be difficult to apply a dose-response relationship because of the wide range of effective levels of the various compounds included. Use general descriptive outlines of the element's effects (CTCP, Merck, basic documents) to generate* a dose-response curve for all compounds. In some cases, thresholds may be set by looking at levels necessary for life	A45

BRANCH H--METALLO-ORGANICS

Enter from A8

Step Number	Start	Next Step Number
H1	This branch was defined only to bring out the differences between metallo-organics and the more usual organic compounds.	H2
H2	Are the sources of the compound principally from human manufacturing and use of the compound per se? Yes No	 A9 H3
H3	Some metallo-organics, e.g., methylmercury, are formed in the environment following the release of metals. From basic documents and limited literature search, estimate* the rate constants, λ_{mo}, for production of the metallo-organic from the metal in air, water, and land. Apply these to the steady state inventories of metals (SSI_m) as estimated in Step A32, to obtain the release rates for the metallo-organic: $R_{mo} = \lambda_{mo} SSI_m$	H4
H4	Any problems? Yes No	 Z1 H5
H5	Similarly, estimate the media half-lives of the metallo-organic with respect to both removal to relatively inaccessible reservoirs and transformation back into metallic or other forms.	A32

BRANCH I--INORGANICS

Enter from A8

Start

Step Number		Next Step Number
I1	This branch was defined to bring out the differences between inorganics and organics.	I2
I2	Production information is usually found in MY, Census, CEH. Otherwise go to AA1 and return to.	I3
I3	Similar instructions apply to imports and exports (see also AB1)	I4
I4	Similar instructions apply to intermediate and dispersive uses (see also AC1).	I5
I5	Complete Steps A15-A20, using above sources and Anderson (1973).	I6
I6	Complete Steps A21 and A22	I7
I7	Any problems in Steps I2-I6? Yes.	Z1
	No	I8
I8	Examine information on transformations of the compound in the environment. For example, sulfur dioxide passes through several stages of transformation to become relatively innocuous neutral sulfates (e.g., ammonium sulfate). Estimate* environmental half-lives on the basis of these transformations and other movements to relatively inaccessible reservoirs.	A32

BRANCH J--HALF-LIVES

Enter from A24, A27, A30, L5

Start

Step Number		Next Step Number
J1	For the medium in question, determine from the basic documents and chemical reasoning whether	
	the chemical is unlikely to disappear rapidly	J2
	the chemical is likely to disappear rapidly	J3
	there is no basis for judgment.	J4
J2	T_x = 10 yr.[1]	J5
J3	T_x = 0.1 yr.	J5
J4	T_x = 1 yr.	J5
J5	Return at exit point + 2	A26 A29 A32 L6

---

[1] x = A, W, or L; or AW, WL, and so on.

BRANCH K--NONSTEADY-STATE

Enter from A34

Step Number | Start | Next Step Number

K1 This branch makes imprecise but potentially significant adjustments in the "steady-state" inventory estimate for conditions that depart substantially from the steady state. The estimates are based on approximations that should lead eventually to estimates of the average concentrations over the next 5 years. The departure can be determined on the basis of several conditions. Is the determination based on

Growth of releases?. K2
Curtailment of releases?. K3
Long half-life?. K4
Other?. K5

K2 Estimate the doubling time, T_2, in years, and the time that releases have been extant, T. Select correction factor (F) from graph.†. .K6

K3 Estimate the time for which releases have been curtailed, T, and previous release rate, R'. Compute correction factor as:[1]

$$CF = 1 + \frac{T_x}{3.5} (R'/R - 1) \left[e^{-\lambda T} - e^{-\lambda (T+5)}\right] \quad . . . . .K6$$

K4 Estimate the time for which releases have been relatively constant, T. Compute correction factor:

$$CF = 1 - \frac{T_x}{3.5} \left(1 - e^{-\lambda T}\right) \quad . . . . .K6$$

K5 Is the adjustment obvious?
Yes. K6
No Z1

K6 Multiply SSI by CF to obtain new SSI A35

---

[1] T_x = half-life, T_A, T_W, or T_L; $\lambda = 0.693/T_x$.

BRANCH L--INTERMEDIA TRANSFERS

Enter from A36

Step Number	Start	Next Step Number
L1	Estimate, from basic documents a limited literature search, the transfer rates between the various media, and calculate better values for the SSIs.[†]	L2
L2	Any success? Yes. . . . . No	L7 L3
L3	Use the methods described in the instructions (see discussion L1) to estimate the λs from basic considerations, and perform the calculations	L4
L4	Any success? Yes. . . . . No	L7 L5
L5	Use the default values in Branch J then return to L6.	J1
L6	Make the calculations.	L7
L7	Return to	A37

BRANCH M--SPECIAL POPULATIONS

Enter from A38

Start

Step Number		Next Step Number
M1	Here, look for populations at risk that obtain their exposures through means other than general exposure to air (e.g., breathing), water (e.g., drinking), and land (e.g., plant uptake). Some obvious examples of special populations for mercury are fish eaters, cosmetic users, and painters. However, the first two are controlled by other agencies (FDA) and possibly the third also (OSHA). We, on the other hand, are trying to identify special populations at risk that are exposed through means controllable by EPA. For example, the PCB problem was highlighted by the poisoning of chickens eating food contaminated by a heat-exchanger leak. Authority over such incidents is not clear, but conceivably belongs to EPA	M2
M2	Describe,* from basic documents and literature survey, any special populations by their size (N_{SP}) and the distribution of exposures by route of exposure. For example, 20% of N_{SP} might have exposures averaging X/2, 60% at X, and 20% at 2X	M3
M3	Any problems? Yes	Z1
	No	M4
M4	Return to	A39

BRANCH Q--BIODEGRADATION

Enter from A31

Step Number	(Start)	Next Step Number
Q1	Determine, by literature search or simple experiment, the BOD_5 and COD for the chemical.	Q2
Q2	Estimate the biochemical half-life in years by $T_B = 10^{-2}/\ln \frac{COD}{COD-BOD_5}$ where COD is expressed in mg/l oxygen per mg/l chemical concentration, and BOD_5 is expressed in the same units (in the limit as concentration goes to zero)	Q3
Q3	Recompute the water and soil half-lives by $\frac{1}{T_W} = \frac{1}{T_W} + \frac{1}{T_B}$ $\frac{1}{T_L} = \frac{1}{T_L} + \frac{1}{T_B}$	A32

BRANCH S--NONBIOLOGICAL EFFECTS

Enter from A40

Start

Step Number		Next Step Number
S1	Determine whether the effects are	
	physical/chemical corrosion, abrasion, and so on, of man-made things	SA1
	aesthetic in nature, affecting such properties as visibility, color, odor, taste, texture, scale, and so on	SB1
	impairment of resources (e.g., excess salinity for industrial uses of water).	SC1
	other	S2
S2	Are the description and quantification of the effects obvious?* Yes.	S3
	No	Z1
S3	Prepare quantitative description of effects by number and kind	S4
S4	Effects valued in Table A46? Yes.	S5
	No	V1
S5	Multiply numbers of effects by values to obtain ranking indexes. Add to obtain hazard ranking index. Return at	A48

BRANCH SA--EFFECTS ON PROPERTY

Enter from S1

Step Number	Start		Next Step Number
SA1	Construct* a model of the distribution of the items affected by their exposure to the agent. For example, most statuary is in big cities, and most sulfuric acid mist is associated with urban industries. Thus the appropriate dilution factors are relatively small.		SA2
SA2	Any problems?	Yes	Z1
		No	SA3
SA3	Is there enough information in the basic documents to suggest a dose-effect relationship?	Yes	SA4
		No	F1
SA4	Express information in terms of a graph of fractional damage versus dose (e.g., kg/m^3). Integrate damage by distribution of dose from model		SA5
SA5	Does the property in question have clear* economic value?	Yes	SA6
		No	SA7
SA6	Multiply the economic value of all property by the integrated percent damage.		A46
SA7	Is the value of the damaged property essentially* noneconomic, e.g., art?	Yes	SA9
		No	Z1
SA8	Return to		A46
SA9	Use the percent damage/yr		A46

BRANCH SB--AESTHETIC EFFECTS

Enter from S1

Step Number	Start		Next Step Number
SB1	From basic documents or limited literature search, establish the threshold of concentration above which the presence of the agent is significantly distasteful (e.g., ppm of SO_2 for visibility, ppm of phenol for taste, size factor for scale).		SB2
SB2	Any problems?	Yes	Z1
		No	SB3
SB3	Construct* a model of the number of people annoyed X times per year, as a function of X. Integrate the people over the frequency distribution to get the number of cases per year.		SB4
SB4	Any problems?	Yes	Z1
		No	A46
SB5	Return to		A46

BRANCH SC--RESOURCE EFFECTS

Enter from S1

Start

Step Number			Next Step Number
SC1	From basic documents[1] or limited literature search, establish the threshold of concentration in the resource that prohibits effective use of the resource (e.g., ppm dissolved solids in water prevent its use as wash water)		SC2
SC2	Any problems?	Yes	Z1
		No	SC3
SC3	Construct* a model of the percent of the resource use denied by the distribution of concentrations. Determine the total economic value of the resource use, e.g., from Manufacturing Value Added (MVA) estimates of the Census of Manufactures. Determine economic loss by multiplying these quantities		SC4
SC4	Any problems?	Yes	Z1
		No	A46
SC5	Return to		A46

---

[1] For example, Water Quality Criteria.

BRANCH V--VALUATION

Enter from A46, CA6, CAA5, CB9, S4

Step Number	Start	Next Step Number
V1	Valuation is an inescapably subjective component of this system. EPA must set the value of any given effect relative to others, or at least concur with the operator's evaluation. A table of values (see Table A46) has been developed for some of the commonly incurred pollutant effects. For the effect under consideration, determine a value per case relative to those in the table. For example, the value of a given decrement in visibility due to particulate matter in the air would presumably be about equal to that for the visibility effects of NO_2. Or one might compute the economic penalties of hair loss, say, by looking at physician diagnostic costs and the price of hairpieces, and then comparing them with the economic penalties of crop losses from air pollution to arrive at a value. It will be difficult to fix a value within an order of magnitude, but it is important to try.	V2
V2	Any insurmountable problems? Yes	Z1
	No	V3
V3	Add value(s) to Table A46. Return to former branch at next stop	A47 CA7 CAA6 CB10 S5

BRANCH Z--AD HOC STUDIES

Enter from AA7, AA11, AB3, AF2, AG2, CAA2, CAA4, CAB3, CABC5, CB4, E4, G6, H4, I7, K5, M3, S2, SA2, SA7, SB2, SB4, SC2, SC4, V2

Step Number	Start	Next Step Number
Z1	Prepare brief document describing problem area. Prepare materials on appropriate* portions of ranking procedure, with examples. Identify expert in area, inside or outside EPA. Request ad hoc provision of information leading to next step. Budget $1,000 or less	Z2
Z2	Return to next step	AA8 AA12 AB4 AF3 AG3 CAA3 CAA5 CAB4 CABC6 CB5 E5 G7 H5 I8 K6 M4 S3 SA3 SA8 SB3 SB5 SC3 SC5 V3

WORKSHEETS AND EXPLANATORY MATERIAL FOR OBJECTIVE PROCEDURE

(Keyed to the Step in the Procedure
to Which They Apply)

Preceding page blank

AGENT NAME ______________________________

BRANCH

Enter step numbers encountered in ranking agent. If sequential, use nomenclature like A3-A7. Use each column for a different branch. It is often useful to place Branch A near the center.

A1 TRACE OF PROCEDURE

Preceding page blank

A2--AGENT IDENTIFICATION

Fill in applicable sections

Agent Name ____

Common Synonyms[1] ____

____

____

☐ Chemical ☐ Physical ☐ Radiological

☐ Biological ☐ Other

For chemical agents:

☐ Compound ☐ Element ☐ Mixture

CAS Registry No.[1] ____________________

Molecular Formula[1] ____________________

Structural Formula[2]:

Melting Point[3] __________ °C

Boiling Point[3] __________ °C

Vapor Pressure[3] @20°C ______ mmHg

Density[3] @ 20°C __________ Kg/l

Water Solubility,[3] 20°C ______ Kg/l

Partition Coefficient[4] ______

For physical agents:

☐ thermal ☐ particulate ☐ solid waste ☐ Other

Description/definition: ______________________________

____

____

Temperature ______________ °C (for thermal agents)

Density ______________ Kg/l } (for particulates)

Particle Size ______________ microns }

A2--Concluded

For radiological agents:

☐ alpha ☐ beta ☐ gamma or x-ray ☐ mixed ionizing

☐ ultraviolet ☐ visible ☐ infrared and microwave

For non-ionizing: Frequency range ________________ Hz

For ionizing: Mean quantum energy ____________ Mev

For biological agents:

☐ viral ☐ bacterial ☐ rickettsial

☐ protozoan ☐ higher forms

Species included ____

____

____

Typical Size ______________________________________ microns

Notes:

1 CHEMLINE, TADS, TSL

2 Merck, SOCMA

3 TDB, HPC, Lange, If not found, estimate to one decimal accuracy by comparison

4 CR

A4--EFFECTS CHECKLIST

Agent Name ____

Check the suspected effects

Human: ☐ Mortality through ____________________
☐ Serious disease or injury ____________________
☐ Other disease or injury ____________________
☐ Physiological effects ____________________
☐ Aesthetic impact through ____________________
☐ Economic impact through ____________________

Animal: ☐ Mortality through ____________________
☐ Reproduction impairment through ____________________
☐ Yield reduction through ____________________

Plant: ☐ Mortality through ____________________
☐ Reproduction impairment through ____________________
☐ Yield reduction through ____________________

Other: ☐ Ecosystem disturbances through ____________________

Describe the principal concern: ____

____

____

____

____

This worksheet and worksheet A2 should be reviewed with the nominator before major ranking steps are undertaken.

A13--INTERMEDIATE AND DISPERSIVE USES

When a chemical is used in reactions to form other chemicals, such use is called "intermediate use." All other uses, whether industrial, commercial, or in consumer products, are dispersive. The distinction becomes tenuous when the chemical is reacted before, during, or shortly after its dispersive use, for example when adhesives polymerize and set, or when bleaches oxidize colorants. However, these latter uses are usually considered to be dispersive.

By definition, dispersive uses (DU) and intermediate uses (IU) account entirely for the net disappearance of a chemical:

$$DU + IU = P + I - E$$

It is the dispersive uses that are of environmental concern, and they can be estimated either directly or by determining P, I, E, and IU.

IU is estimated by examining all the processes that use the chemical to make others, and by estimating the consumption in each. The most comprehensive source of this information, even though it covers only a few hundred compounds, is the Chemical Economics Handbook (CEH).

However, DU can be estimated directly by examining all the products and activities that the chemical is used for. This information is also often found in the CEH. If the major uses all fall into the following list, then the NCI data bank is also useful: food additives, drugs, cosmetics, soaps and detergents, paints. Dispersive use estimates can also be found for 80 compounds in NSF, and for others in COM and the basic documents.

A20--RELEASE WORKSHEET

Agent Name ______________________________

☐ produced commercially ☐ other human sources[1]

P ____________________ kg/yr production

I ____________________ kg/yr imports

E ____________________ kg/yr exports

IU ____________________ kg/yr intermediate uses

DU ____________________ kg/yr dispersive uses

(P + I - E - IU ☐, or directly ☐)

	Releases during production (fractional)	Releases during use (fractional)
Air	e_A ________	f_A ________
Water	e_W ________	f_W ________
Land	e_L ________	f_L ________

Release Rate Computation

	Production	Use	Trans-portation	Other	Total	
Air	$P \times e_A =$ ______	$+ DU \times f_A$ ______	+ ______	+ ______	= ______	kg/yr
Water	$P \times e_W =$ ______	$+ DU \times f_W$ ______	+ ______	+ ______	= ______	kg/yr
Land	$P \times e_L =$ ______	$+ DU \times f_L$ ______	+ ______	+ ______	= ______	kg/yr

Derivation of Estimates (Document with brief narrative)

Production Processes

____

____

____

---

[1] Includes combustion products, release during other activities as waste, and so on. May be available in basic documents or calculable from EF.

A20--Concluded

Intermediate Uses

Dispersive Uses

Transportation Releases

Other Releases

A22--LOCATION OF POTENTIAL RELEASES TO ENVIRONMENT

Production

Firm	Location	Quantity Produced per Year	% of Total

Consumption (Nondispersive Uses)

Firm/Industry	Location	Quantity Used per Year	% of Total Produced

Consumption (Dispersive Uses)

Firm/Industry	Location	Quantity Used per Year	% of Total Produced

A22--Continued

Transportation

Firm/Industry	Type of Carrier	Quantity Carried per Year	% of Total Produced

Storage

Firm/Facility	Container	Mean Quantity Stored	Mean Residence Time

Natural Sources

Phenomenon/ Ecosystem	Location	Quantity Released per Year

A22--Concluded

Natural Sinks

Phenomenon/ Ecosystem	Location	Quantity Absorbed per Year

Complete outline maps if appropriate. See The National Atlas of the United States (U.S.G.S.) for outline maps of administrative subdivisions for individual federal agencies if necessary.

A25--AIR OXIDATION

Oxidation and/or the photochemical degradation are the major sources of degradation in the atmosphere. The dominant fate is oxidation, with photochemistry usually resulting in oxidation products. Direct photolysis is usually of minimal consideration, because most compounds absorb below the 300 nm solar region cut-off. In the evaluation of oxidation under environmental conditions for NSF-RANN, SRI considered ozone (O_3) and the hydroxyl radical (•OH) as the primary air oxidants; both have been demonstrated to be important in air pollution modeling. Although concentrations of these species are subject to environmental conditions (sunlight intensity, other pollutants present); they can be estimated correctly within an order of magnitude that is useful for kinetic predictions.

Ozone is formed by photochemical processes in nature and is also derived from direct and indirect anthropogenic sources. The harmful effects and reactivity of ozone are well demomstrated. Data on the rates of reactions of ozone are reasonably available for calculations. We assign an ambient concentration of 0.05 ppm (about 2×10^{-9})M).

The hydroxyl radical is a very reactive species and is of pivotal importance in all air pollution modeling systems. Ambient concentrations of 10^{-15} M are assigned for these calculations.

In air, the oxidation of a chemical may then be represented as

$$-\frac{d(\text{chemical})}{dt} = \left[k_{\cdot OH}[\cdot OH] + k_{O_3}\left[O_3\right]\right][\text{chemical}]$$

The values of k_{OH} and k_{O_3} ($M^{-1}\ sec^{-1}$) are based on available literature information, either for the compound directly, or by analogy to other appropriate compounds for which data are available. A half-life (seconds) in the atmosphere may then be approximated by:

A25--Concluded

$$T_A = \frac{0.693}{k_{OH}[OH] + k_{O_3}\left[O_3\right]}$$

The half-lives should then be converted from seconds to years.

A28--WATER DEGRADATION

Both oxidation and hydrolysis may degrade a chemical in the aquatic environment. Oxidation in this phase was estimated for the NSF-RANN study by assuming alkyl peroxyl radicals ($RO_2\cdot$) as the active oxidant species, because these radicals are readily regenerated in the presence of oxygen. A concentration of 10^{-10} M was assigned, using a solar flux value of 2.2×10^{-7} einsteins/cm^2sec, with acetone as a representative photosensitizer, and a product quantum yield of about 10^{-2}. With this concentration and the large amount of kinetic data on alkyl peroxyl radical reactions, the oxidation in water can be estimated.

Hydrolytic degradation of a compound may be accelerated by both acidic and basic conditions. For most compounds, a minimal rate of hydrolysis will occur at pH ~ 7, and we suggest referencing all data to this value. Extrapolation of data to this pH is reasonable, and some data are available in the literature for this pH. However, no comprehensive review of literature data on hydrolysis is available at this time. Although there is little information directly relevant to an environmental assessment, there is a large amount of data on hydrolysis at higher temperatures and in various solvent systems. These data may be extrapolated or rendered useful through use of various empirical and theoretical calculation techniques currently accepted by physical organic chemists.

As with the air oxidation degradation, the disappearance of a compound in the aquatic environment may then be represented by

$$-\frac{d(\text{chemical})}{dt} = \left[k_{RO_2\cdot}\left[RO_2\cdot\right] + k_h\right][\text{chemical}]$$

where k_{RO_2} is a biomolecular rate constant (M^{-1} sec^{-1}) and k_h is the pseudo-first order rate constant (pH = 7) in sec^{-1}.

A28--Concluded

An aquatic half-life in seconds may then be calculated by

$$T_W = \frac{0.693}{k_{RO_2\cdot}\left[RO_2\cdot\right] + k_h}$$

The half-lives should then be converted from seconds to years.

A31--COMPUTATION OF LAND HALF-LIVES

Simple and wholly objective predictors of residence times in soils are either unavailable, or, as in the case of Lambert's use of parachor, untested for many classes of agents. Hence, informed speculation remains the only consistently applicable method for predicting residence times in soils.

However, objective estimates can be obtained for selected groups of chemicals. For example, sorption rates and parachor are strongly correlated for pesticides, and this correlation, if calibrated against chemicals of known residence times, potentially could be used to obtain an estimate of residence times.

Clearly, the more rapid the sorption, the longer the residence time in unavailable forms is likely to be, and conversely the shorter the residence time is in soluble forms.

With the surface tension, γ, in g/sec^2 and the density ρ, in g/cm^3, the parachor, P, is given by

$$P = M\,\gamma^{1/4}/\rho$$

where M is the molecular weight.

The equilibrium constant, K_e, between liquid and solid phase is then estimated by

$$K_e = 0.2e^{0.0125\,P}$$

The half-life for movement from the liquid (ℓ) to the solid (s) phase is related to that for movement back into the liquid phase by

A31--Concluded

$$T_{\ell \rightarrow s} = T_{s \rightarrow \ell}/K_e$$

Assuming that the concentration in the solid phase never reaches equilibrium with that in the liquid phase, the net half-life in the liquid phase is given by

$$T_L = \frac{T_{s \rightarrow \ell}}{K_e - 1}$$

We finally assume that $T_s \rightarrow \ell$ is very long, arbitrarily 50 years. Therefore, T_L in years is given by

$$T_L = \frac{50}{K_E - 1}$$

Since only the liquid phase is environmentally available, T_L is the land half-life.

A32--TRANSPORT/TRANSFORMATION WORKSHEET

Agent Name ____

1. Chemical Transformation (Steps A25-A31)

Air: k_{OH} _____ $(Yr)^{-1}$/mole k_{O_3} _____ $(Yr)^{-1}$/mole T_A _____ Yr

Water: k_{RO_2} _____ $(Yr)^{-1}$/mole k_h _____ $(Yr)^{-1}$/mole T_W _____ Yr

Soil: P _____ K_e _____ T_L _____ Yr

2. Intermedia Transfer (Step A35)

Transfer rates, in $(Yr)^{-L}$, from column heading to row heading

	Air	Water	Land
Air	— _________	_________	_________
Water	_________	— _________	_________
Land	_________	_________	— _________

3. Steady State Inventory (Step A32)

Solve equations shown in discussion L1

R_A _______ kg/yr SSI_A _______ kg

R_W _______ kg/yr SSI_W _______ kg

R_L _______ kg/yr SSI_L _______ kg

4. Non-steady State Correction (Step A33)

CF_A _______ SSI_A _______ kg

CF_W _______ SSI_W _______ kg

CF_L _______ SSI_L _______ kg

5. River/Lake Partition (see discussion A39)

Lakes f _________ SSI _________ kg

Rivers f _________ SSI _________ kg

A32--Concluded

6. Concentrations (Step A39)

	Dilution Factors, D	Fraction of SSI, f_D	Concentration[1]
Air	10^6 m^3		kg/m^3
	10^8 m^3		kg/m^3
	10^{10} m^3		kg/m^3
	10^{12} m^3		kg/m^3
	10^{14} m^3		kg/m^3
	10^{16} m^3		kg/m^3
Rivers	10^{11} l		kg/l
	10^{12} l		kg/l
	10^{13} l		kg/l
	10^{14} l		kg/l
	10^{15} l		kg/l
Lakes	3×10^6 l		kg/l
	3×10^8 l		kg/l
	3×10^{10} l		kg/l
	3×10^{12} l		kg/l
	3×10^{14} l		kg/l
	3×10^{16} l		kg/l
Land	5×10^6 m^2		kg/m^2
	5×10^8 m^2		kg/m^2
	5×10^{10} m^2		kg/m^2
	5×10^{12} m^2		kg/m^2

---

[1] If release rate and/or transformation rate data are inadequate, use ambient concentrations observed, from SAROAD and STORET.

A37--POPULATIONS AT RISK

Human

	Name of Group	Estimate Size of Group
• Geographic groups (e.g., Northeastern U.S. central city dwellers)	____________	____________
	____________	____________
	____________	____________
	____________	____________
• Occupational groups[1] (e.g., farmers)	____________	____________
	____________	____________
	____________	____________
	____________	____________
• Avocational groups (e.g., fishermen)	____________	____________
	____________	____________
	____________	____________
	____________	____________
• Dietary groups[1] (e.g., Weight-Watchers)	____________	____________
	____________	____________
	____________	____________
	____________	____________
• Other (e.g., socio-economic groups)	____________	____________
	____________	____________
	____________	____________
	____________	____________

---

[1] Prime responsibility generally is that of other agencies.

A37--Concluded

	Name	Location	Number at Risk
Domestic or Captive Nonhuman			
• Livestock (e.g., dairy cattle; minks)			
• Pets (e.g., cats; goldfish)			
• Captives (e.g., lions, bears)			
Wild Nonhuman			
• Widespread rare or endangered[1] species			
• Geographically isolated rare or endangered species			

---

[1] Endangered either by the agent of interest or by other means (e.g., changes in land use).

A39--DILUTION FACTORS

Air

We assume that a typical diffusion and transport velocity is about 1 m/sec or 3×10^7 m/yr horizontally, and 10^4 m/yr vertically. We also assume that the agent has about 10^{16} m^3 available for expansion (this limits the expansion to about a 1 km layer over the United States). Thus a puff of agent released would fill this volume within about 1/10 yr.

If the agent remained in the air a relatively long time (>1 yr), a steady state would result in a relatively uniform distribution of concentrations, with only a slight peaking near points of release; this is because the total inventory would be large in comparison with the release rate. For shorter half-lives, the gradient of concentrations away from the release point would be larger, because the agent would not exist long enough to diffuse to the limits.

A rough calculation results in Table A39.1, which shows the percentage of the steady-state inventory that is in various dilution volumes as a function of half-life. Interpolation on log-log paper is permissible.

Table A39.1

PERCENTAGE OF SSI IN VOLUME INDICATED (AIR)

Dilution Factor (m^3)	Half-Life (yr)				
	10^{-3}	10^{-2}	10^{-1}	10^{0}	10^{1}
10^6	5×10^{-4}	6×10^{-7}	3×10^{-7}	1×10^{-8}	1×10^{-8}
10^8	4×10^{-2}	6×10^{-5}	3×10^{-5}	1×10^{-6}	1×10^{-6}
10^{10}	2.1	5×10^{-3}	2×10^{-3}	1×10^{-4}	1×10^{-4}
10^{12}	37	4×10^{-1}	2×10^{-1}	1×10^{-2}	1×10^{-2}
10^{14}	60	13	2	1	1
10^{16}	1	86	98	99	99

Water

The same general principles hold for water as for air, but the likely transport rates and dilution volumes are quite different. All agents released into water can eventually reach the ocean, but they are relatively unlikely to move from one river system to another, for example.

The total flow of all rivers in the United States is about 2×10^{15} l/yr; in a case of uniform steady state for long-lived agents, this would be the dilution factor because all of the annual input would reach the ocean. We assume that the velocity of turbulent diffusion is about 100 m/hr, or about 10^6 m/yr, and that river dimensions are typically 100 m by 10 m. Therefore uniform mixing across the rivers occurs within hours, and only extremely short-lived agents ($T_W < 10^{-4}$ yr) would not be mixed. On the other hand, flows are typically 5 km/hr or 5×10^7 m/yr, and river lengths are typically 1,000 km (10^6 m). Consequently, a similar table (A39.2) can be constructed for water dilution factors.

Table A39.2

PERCENTAGE OF SSI IN VOLUME INDICATED (RIVER WATERS)

Dilution Factor (l)	Half-Life (yr) 10^{-3}	10^{-2}	10^{-1}	10^{0}
10^{11}	1×10^{-2}	1×10^{-2}	1×10^{-2}	1×10^{-2}
10^{12}	1	9×10^{-2}	9×10^{-2}	9×10^{-2}
10^{13}	12	1.3	9×10^{-1}	9×10^{-1}
10^{14}	62	16	10	9
10^{15}	25	82	89	90

A39--Continued

Note that rivers of the size assumed here would empty 50 times per year, for a total volume of 5×10^{13} 1. It would take 400 rivers of such size to supply the total runoff indicated above. If it is suspected that only N rivers are significantly contaminated, then the dilution factors on Table A39.2 should each be multiplied by N/400 before further analyses proceed.

The total volume of all lakes and ponds in the United States, including all of the Great Lakes, is about 3×10^{16} 1. This represents an area of about 4×10^{11} m^2 times an average depth of about 75 m. We estimate that mixing occurs at a rate of about 10 m/hr horizontally and about 100 m/yr vertically. Since few lakes have dimensions greater than 100 km wide or 100 m deep, complete mixing usually takes place within a year. Transport in lakes is more like transport in air than it is like transport in rivers, so we use a scaled version of Table A39.1 for lakes (see Table A39.3).

Table A39.3

PERCENTAGE OF SSI IN VOLUME INDICATED (LAKE WATERS)

Dilution Factor (1)	Half-Life (yr)				
	10^{-2}	10^{-1}	10^{0}	10^{1}	10^{2}
3×10^{6}	5×10^{-4}	6×10^{-7}	3×10^{-7}	1×10^{-8}	1×10^{-8}
3×10^{8}	4×10^{-2}	6×10^{-5}	3×10^{-5}	1×10^{-6}	1×10^{-6}
3×10^{10}	2.1	5×10^{-3}	2×10^{-3}	1×10^{-4}	1×10^{-4}
3×10^{12}	37	4×10^{-1}	2×10^{-1}	1×10^{-2}	1×10^{-2}
3×10^{14}	60	13	2	1	1
3×10^{16}	1	86	98	99	99

If it is known that discharges occur only into lakes of total volume V, then the dilution factors should be scaled by $V/3 \times 10^{16}$ and the half-lives by $(V/3 \times 10^{16})^{1/3}$.

Sometimes the relative discharges into lakes and rivers are known, and the fraction, f, of the inventory in each can be assumed to be the same. If this division is not known, assume it is 50-50.

A41--BIOLOGICAL EFFECTS CHECKLIST

Agent Name ____

Species at risk: (select no more than 5)

☐ Man ____________________
☐ Domestic animals ____________________
☐ ____________________
☐ Other animals ____________________
☐ ____________________
☐ ____________________
☐ Crops ____________________
☐ ____________________
☐ ____________________
☐ Other plants ____________________
☐ ____________________
☐ ____________________

Effects to be considered: (select[1] no more than 3 for men, 1 each for other species)

Species	Effects	Indicator Test[2]
Man		

---

[1] Selection should be based on suspected dominance of value once ranking is complete.

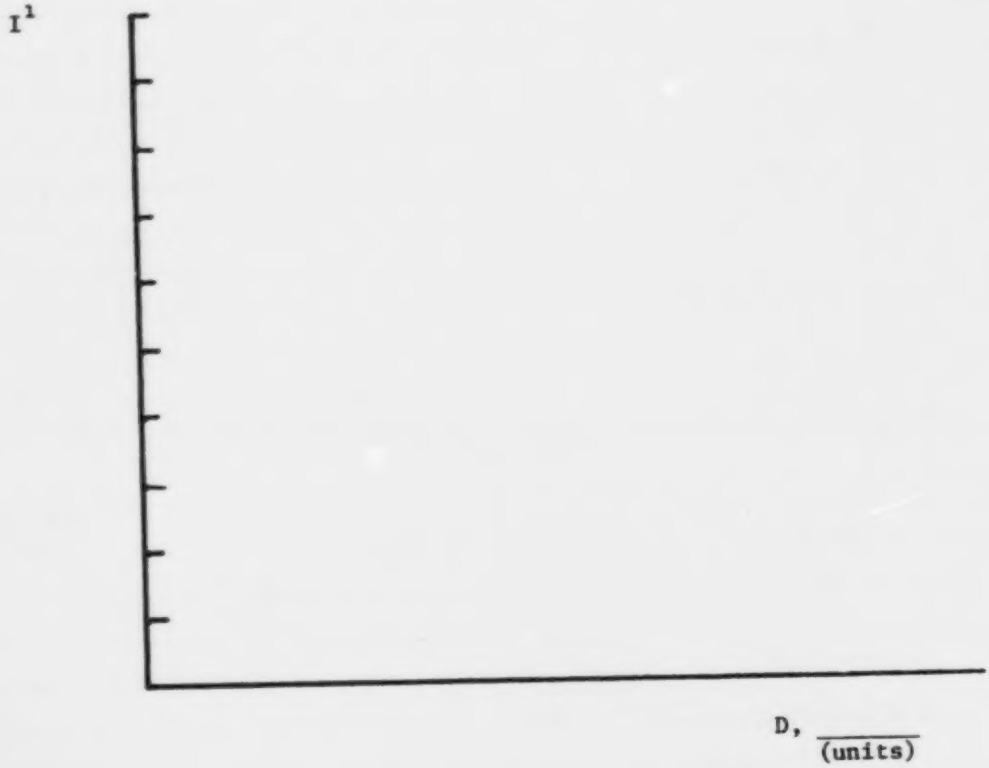
[2] For example, LD_{50} (mouse), human epidemiology, or TLV.

A45--DOSE-EFFECTS WORKSHEET

Agent Name ____

Effect _____________________ in species ________ ___________

Dose-response relationship:



Justification: ____

____

____

____

____

---

[1] Incidence, fractional, of effect at dose shown. Enter scale as required (maximum 1.0). Excess over background is implied.

A45--Concluded

N_i Number at Risk[1]	C Concentration /Units	E Exposure[2] Factor/Units	D=CxE Dose /Units	D' Converted Dose/Units	I_i Incidence	NC_i Cases
					Total Cases	

In some cases it may be simpler to express the exposure dose information as a distribution, dN/dD (number per unit dose) as a function of D. The number of cases is then given by

$$NC = \int_{\text{Threshold}}^{\text{Saturation}} \frac{dN}{dD} (D)\ I\ (D)\ dD$$

---

[1] Absolute number or percent of total population (show with %). See also high dose distribution discussion, A45.2.

[2] See Table 45.1, BDB, Altman, Prosser, or Dill.

A45--Concluded

Table A45.1

EXPOSURE FACTORS[1]

Species	Weight, kg	Food Intake, kg/yr	Water Intake,[2] l/yr	Air Intake,[3] m^3/yr
Man	65	550	450	7,000
Monkey	5	90	--	850
Dog	10	275	350	2,000
Cat	2	37	--	800
Cattle	500	2,750	17,000	60,000
Horse	500	3,650	8,000	35,000
Sheep	60	875	1,000	8,000
Rabbit	2	22	125	450
Rat	0.4	7	12	280
Mouse	0.02	1	2.5	35
Chicken	2	90	--	600

---

[1] Use these values with caution, they are subject to many caveats. Although they are adequate for the purposes of this ranking, they should not be used for more demanding tasks, such as the development of the STARS.

[2] Drinking, doesn't include water in food or water of metabolism.

[3] Tidal Volume--not all is taken in by far (about 8% of the oxygen in the tidal volume is).

A45.2--HIGH DOSE DISTRIBUTION

Because the procedure in Step A39 computes single concentration value for discrete populations, rather than a continuous distribution, the highest concentration is often below the threshold for toxic effects. Consequently, the hazard index is estimated as zero, and no discrimination is made between agents with concentrations near the threshold and those with concentrations far below it. (When a zero threshold is assumed, this problem does not arise.)

If the highest predicted concentration does, in fact, fall below the threshold for a given effect, the possibility that smaller numbers of the exposed population are receiving even higher doses should be explored. This could occur, for example, during rare but significant incidents of accidental exposure, such as chemical spills.

If such a possibility exists, the suggested procedure is to assume that the number of people (or other organisms at risk) varies inversely with doses above the highest dose predicted from Step A39. Let the highest predicted dose by D_h, and the number exposed to that dose be N_{ih}. Then the number exposed to a higher dose D is estimated by

$$N = N_{ih} D_h / D$$

If the threshold dose is D_t, choose two or three doses higher than D_t at which to estimate N. Ordinarily, it is convenient to choose doses spaced by a factor of 10, following the pattern of Step A39, then combine with these dose/number combinations as in Step A45. In some cases it may be desirable to extrapolate from some other high A39 dose D_h, and compare the resulting N's for the same D's with those from the first extrapolation.

A46--VALUATION

Valuation is surely the most controversial part of an "objective" ranking system. We recommend that the values suggested here be examined closely by the operator and replaced where necessary. When in doubt, complete a sensitivity analysis.

Effect	Examples	Units	Value/ Unit
Excess human mortality	Terminal cancer, acute poisoning	Deaths/yr	1,000
Excess human morbidity Serious disease	Cancer, heart disease, chronic respiratory disease, chronic kidney or liver disease	Cases/yr	200
Excess human morbidity Other disease	Acute respiratory disease, hay fever dermatitis	Cases/yr	10
Life shortening	Lower life expectancy in irradiated population	Yr/yr	50
Physiological effects of uncertain significance	Proteinurea	Occurrences/yr	1
Aesthetic annoyance	Observation of solid waste in water, odor annoyance	Occurrences per person/yr	1
Economic losses	Excess painting, loss of industrial production	Dollars/yr	.01
Mortality in domestic[1] animals	LD_{50} for chickens, LC_{50} for tuna	% of population per year	10,000[2]
Morbidity in domestic animals	Molybdenosis	% of population per year	1,000[2]
Mortality in other animals	Bald eagle, neomysis shrimp	% of population per year	1,000[3]
Loss of yield in crops	Corn, pines	% of yearly harvest	10,000[2]

A46--Concluded

Effect	Examples	Units	Value/ Unit
Mortality in other plants	Seaweed	% of population per year	1,000[3]
Effects on sensitive indicator species	Eggshell thinning	Occurrences/yr	10

---

[1] Supplying major human food needs or significant useful work.

[2] If over 50%, increase value by factor of 3.

[3] If over 50%, increase value by factor of 10.

A47--HAZARD RANKING WORKSHEET

(Page ___ of ___)

Agent Name ____

1. Effect	2. Cases/Units	3. Value	Ranking Index (2. x 3.)

Page Total (Environmental Hazard Index) ______________

Sum of ___ pages (Total Environmental Hazard Index) ______________[1]

Date	Rank[2]

---

[1] Applicable only to last page of multi-page forms.

[2] Enter new rank each time it changes as a result of new entries to the list.

CA5--RADIATION DOSE-EFFECTS RELATIONSHIPS

The following relationships have been used for predicting long-term human health effects of ionizing radiation.

Genetic Deaths

$$N_{gd} = 0.19\ b_1\ D/100$$

where N_{gd} is the number of genetic deaths/yr

b_1 is the number of births/yr

and D is the annual absorbed dose in rad for the reproducing population.

Induced Neoplasms

$$N = N^* \times 10^{-6} \times \frac{D}{D_d} \times P$$

where N is the number of neoplasms/yr

N^* is the number of spontaneous neoplasms per year per million

D is the dose in rads/yr

D_d is the doubling dose in rads

and P is the population.

For thyroid neoplasms only,

$$N = \left[F_o\ N_o^*\ \frac{D_e + D_i}{D_{do}} + F_y\ N_y^*\ \frac{D_e + D_i}{D_{dy}}\right] P \times 10^{-6}$$

where F_o and F_y are the fractions of the population over and under 20 years of age, D_e and D_i are the external and internal doses, and the other parameters are as given below.

CA5--Concluded

Neoplasm	N^*	D_d
Thyroid, o	40	100
y	4	10
Respiratory system	294	175
Digestive system	482	230
Breast	143	100
Lymphatic/ Hematopoietic	83	70
Leukemia	72	50
All	1,500	175

Life Shortening

10 days per rad.

CABA2--ORGAN MASS FOR HUMANS
(kg)

Organ	Newborn	1	3	10	Adult
GI Tract	.13	.31	.60	.85	1.64
Bone	.20	.65	1.17	2.56	7.00
Liver	.13	.32	.48	.83	1.60
Kidneys	.02	.06	.08	.15	.28
Thyroid	.002	.002	.004	.009	.020
Total Body	3.5	11.0	15.0	32.0	65.0

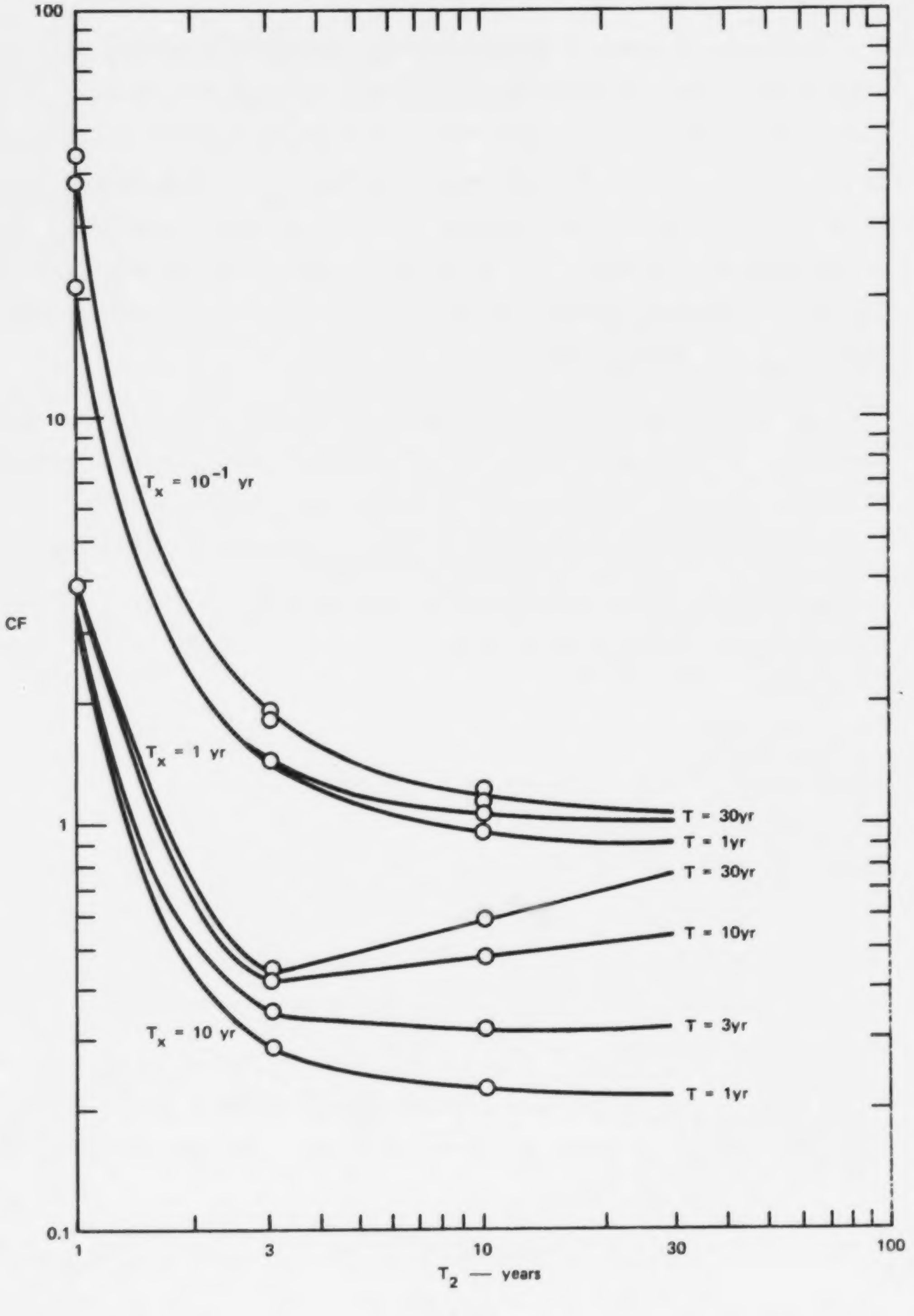
D5--MULTIPLE AGENTS

If agent is represented by several compounds, list them here.

Agent as initially designated or defined ______________________________

Representatives	Reason for Choice

K2 CORRECTION FACTORS FOR NON-STEADY-STATE CONDITIONS



L1--INTERMEDIA TRANSFERS

Physical transfers between two media can markedly affect the steady-state inventories and the concentrations to be expected in each. At first order, we assume that transfer rates are linearly related to inventories in the original medium through rate constants $\lambda_{mm'}$. For example, λ_{AW} would be the transfer rate constant from air to water, whereas λ_{WA} would be the constant for water to air (evaporation). (The transfer rate constants are inversely related to the characteristic half-life for the process: $\lambda_{AW} = 0.693/T_{AW}$, and so on.)

The most common transfers are evaporation (water or land to air), deposition (air to water or land), and sedimentation (water to sediments). In this subsystem, both land and sediments are considered to be parts of a single, relatively inaccessible, reservoir or sink for pollutants.

Evaporation can be estimated by the techniques of Mackay and Wolkoff (1973) if very sweeping assumptions are made. The basic equation suggested is

$$\lambda_{WA} = 230 \frac{M_i P_{is}}{C_{is}}$$

where λ is in $(yr)^{-1}$, M_i is the molecular weight, C_{is} is the solubility in water (mg/ℓ), and P_i is the vapor pressure (mmHg at 20°C). This equation could also be used for land to air evaporation, but with even less certainty. Usually land to air evaporation is ignored, but not always with justification.

Sedimentation is not well understood, but probably varies linearly with solubility, all other things being equal. The equation suggested is

$$\lambda_{WL} = 7{,}000/C_{is}$$

L1--Concluded

In general, deposition rates from air are also difficult to estimate. Gases can be assumed not to deposit, although they can, in fact, adsorb on soil or dissolve in water. Most solid particulates of size greater than 10 microns can be assumed to deposit rather quickly (T_{AW} or T_{AL} of the order of a few hours to a few days). Aerosols and vapors would be intermediate in rate of transfer.

For very low vapor pressure (less than 0.01 mmHg), assume $\lambda_{AL} = 2$ (washout). For vapor pressures between 0.01 and 1, assume $\lambda_{AL} = 0.7$. For vapor pressures between 1 and 100, assume $\lambda_{AL} = 0.07$. For higher vapor pressures, $\lambda_{AL} = 0$.

Because oceanic pollution is disregarded, the significant transfer is assumed to be air to land, and λ_{AW} can usually be ignored.

Once the T's and the corresponding λ's have been estimated, the significant terms of the following three equations should be written down and solved for the SSI's:

$$\left(\lambda_A + \lambda_{AW} + \lambda_{AL}\right) SSI_A - \lambda_{WA} SSI_W - \lambda_{LA} SSI_L = R_A$$

$$- \lambda_{AW} SSI_A + \left(\lambda_W + \lambda_{WA} + \lambda_{WL}\right) SSI_W - \lambda_{LW} SSI_L = R_W$$

$$- \lambda_{AL} SSI_A - \lambda_{WL} SSI_W + \left(\lambda_L + \lambda_{LA} + \lambda_{LW}\right) SSI_L = R_L$$

Use these values instead of those calculated with the simpler equations of Step A32.

Appendix G

SAMPLE RANKING RESULTS FOR CARBON DISULFIDE AND CYANIDES

Preceding page blank

Carbon Disulfide

Preceding page blank

A2 - AGENT IDENTIFICATION

Fill in applicable sections

Agent Name CARBON DISULFIDE

Common Synonyms[1] CARBON BISULFIDE
CARBON SULFIDE
DITHIOCARBONIC ANHYDRIDE

☒ Chemical ☐ Physical ☐ Radiological
☐ Biological ☐ Other

For chemical agents:

☒ Compound ☐ Element ☐ Mixture

CAS Registry No.[1] 75-15-0

Molecular Formula[1] CS_2

Structural Formula[2]: $S=C=S$

Melting Point[3] -110.8 °C

Boiling Point[3] 46.3 °C

Vapor Pressure[3] @20°C ~300 mmHg

Density[3] @ 20°C 1.26 Kg/l

Water Solubility,[3] 20°C 2.2×10^{-3} Kg/l 22°C

Partition Coefficient[4] 100:1

For physical agents:

☐ thermal ☐ particulate ☐ solid waste ☐ other

Description/definition: ______

Temperature ______ °C (for thermal agents)

Density ______ Kg/l (for particulates)

Particle Size ______ microns (for particulates)

Preceding page blank

A4 - EFFECTS CHECKLIST

Agent Name CARBON DISULFIDE

Check the suspected effects

Human: ☒ Mortality through HEART DISEASE
☒ Serious disease or injury HEART DISEASE, CENTRAL NERVOUS SYSTEM
☒ Other disease or injury DEBILITATING
☐ Physiological effects
☐ Aesthetic impact through
☐ Economic impact through

Animal: ☒ Mortality through ACUTE TOXICITY
☐ Reproduction impairment through
☐ Yield reduction through

Plant: ☐ Mortality through
☐ Reproduction impairment through
☐ Yield reduction through

Other: ☐ Ecosystem disturbances through

Describe the principal concern: RECENT WORK HAS INDICATED THAT LOW LEVEL OF CS_2 MAY LEAD TO HEART DISEASE IN HUMANS

This worksheet and worksheet A2 should be reviewed with the nominator before major ranking steps are undertaken.

A20 - RELEASE WORKSHEET

Agent Name CARBON DISULFIDE

☒ produced commercially ☒ other human sources[1]

P 3.5×10^8 Kg/yr production

I 4.5×10^5 Kg/yr imports

E 4.5×10^6 Kg/yr exports

IU 2.6×10^8 Kg/yr intermediate uses

DU 9×10^7 KG/yr dispersive uses

(P + I - E - IU ☒, or directly ☒)

Releases during production (fractional)		Releases during use (fractional)	
Air	e_A 0.05	f_A	1.0
Water	e_W 0.05	f_W	0
Land	e_L 0.05	f_L	0

Release Rate Computation

	Production	Use	Transportation	Other	Total	
Air	$P \times e_A = 1.8 \times 10^7$	$+ DU \times f_A$ 8.3×10^7	+	+ 2×10^7	$= 1.2 \times 10^8$	Kg/yr
Water	$P \times e_W = 1.8 \times 10^7$	$+ DU \times f_W$	+	+	$= 1.8 \times 10^7$	Kg/yr
Land	$P \times e_L = 1.8 \times 10^7$	$+ DU \times f_L$	+	+	$= 1.8 \times 10^7$	Kg/yr

Derivation of Estimates (Document with brief narrative)

Production Processes

HEATING CHARCOAL WITH VAPORIZED SULFUR

---

[1] Includes combustion products, release during other activities as waste, etc. May be available in basic documents or calculable from EF.

A20 (concluded)

Intermediate Uses

RAYON AND CELLOPHANE
CARBON TETRACHLORIDE, OTHER ORGANIC
THIOCARBONATES (RUBBER & PESTICIDES); XANTHATES (RUBBER & PAPER)

Dispersive Uses

SOLVENTS (NOW MOSTLY INDUSTRIAL)
FUMIGANT
WOOD TREATMENT
CORROSION INHIBITION

Transportation Releases

Other Releases

EMISSIONS FROM THE CLAUS SULFUR RECOVERY
(6×10^5 Kg/yr) AND FROM AUTOMOTIVE REDUCING
CATALYTIC CONVERTERS (PERHAPS 10^5) AND IN THE FUTURE,
FROM STATIONARY SOURCE CATALYSTS (PERHAPS 2×10^7 Kg)

A32 - TRANSPORT/TRANSFORMATION WORKSHEET

Agent Name CARBON DISULFIDE

1. Chemical Transformation (Steps A25-A31)

Air: K_{OH} ____ $(Yr)^{-1}$/mole K_{O_3} ____ $(Yr)^{-1}$/mole T_A 0.3 Yr {O ATOM / PHOTO-OXID.

Water: K_{RO_2} ____ $(Yr)^{-1}$/mole K_h ____ $(Yr)^{-1}$/mole T_W ____ Yr

Soil: P ____ K_e ____ T_L ____ Yr

2. Intermedia Transfer (Step A35)

Transfer rates, in $(Yr)^{-1}$, from column heading to row heading

	Air	Water	Land
Air	—	3.5×10^6	6.9×10^3
Water		—	
Land			—

3. Steady State Inventory (Step A32)

Solve ~~[R] = [λ] [SSI]~~ Equations shown in discussion LI

R_A 1.2×10^8 Kg/yr SSI_A 7×10^6 Kg

R_W 1.8×10^7 Kg/yr SSI_W 5×10^2 Kg

R_S 1.8×10^7 Kg/yr SSI_L 2.6×10^3 Kg

4. Non-steady State Correction (Step A33)

CF_A ____ SSI_A ____ Kg

CF_W ____ SSI_W ____ Kg

CF_L ____ SSI_L ____ Kg

5. River/Lake Partition (See discussion A39)

Lakes f .5 SSI 2.5×10^2 Kg

Rivers f .5 SSI 2.5×10^2 Kg NEGLIGIBLE

6. Concentrations (Step A39)

	Dilution Factors, D	Fraction of SSI, f_D	Concentration[1]
Air	10^6 m^3	5×10^{-9}	3.5×10^{-8} Kg/m^3
	10^8 m^3	5×10^{-7}	3.5×10^{-8} Kg/m3
	10^{10} m^3	4×10^{-5}	2.8×10^{-8} Kg/m^3
	10^{12} m^3	3×10^{-3}	2.1×10^{-8} Kg/m^3
	10^{14} m^3	8×10^{-2}	5.6×10^{-9} Kg/m^3
	10^{16} m^3	9×10^{-1}	6.4×10^{-10} Kg/m^3
Rivers	10^{11} l		Kg/l
	10^{12} l		Kg/l
	10^{13} l		Kg/l
	10^{14} l		Kg/l
	10^{15} l		Kg/l
Lakes	3×10^6 l		Kg/l
	3×10^8 l		Kg/l
	3×10^{10} l		Kg/l
	3×10^{12} l		Kg/l
	3×10^{14} l		Kg/l
	3×10^{16} l		Kg/l
Land	5×10^6 m^2		Kg/m^2
	5×10^8 m^2		Kg/m^2
	5×10^{10} m^2		Kg/m^2
	5×10^{12} m^2		Kg/m^2

---

[1] If release rate and/or transformation rate data are inadequate, use ambient concentrations observed, from SAROAD and STORET.

A41 - BIOLOGICAL EFFECTS CHECKLIST

Agent Name CARBON DISULFIDE

Species at risk: (select no more than 5)

- ☒ Man
- ☐ Domestic animals
- ☐
- ☐ Other animals
- ☐
- ☐
- ☐ Crops
- ☐
- ☐
- ☐ Other plants
- ☐
- ☐

Effects to be considered: (select[1] no more than 3 for men, 1 each for other species)

Species	Effects	Indicator Test[2]
Man	CARDIOVASCULAR DISEASE	EPIDEMIOLOGY

---

[1] Selection should be based on suspected dominance of value once ranking is complete.

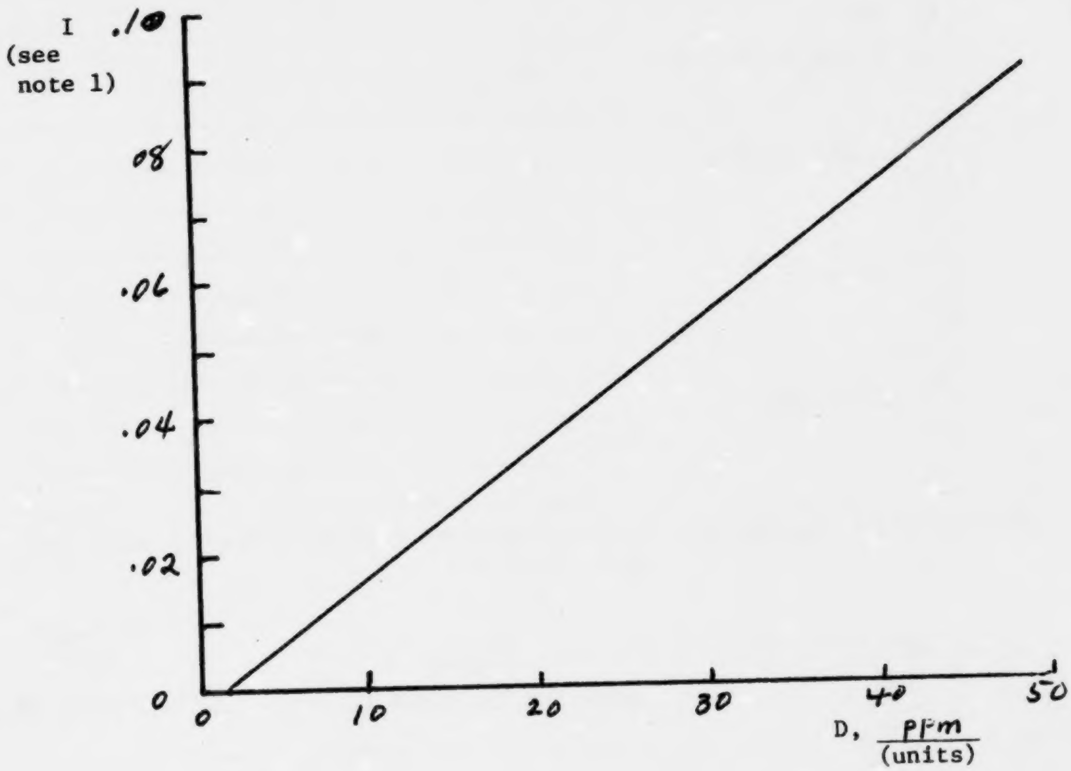
[2] For example, LD_{50} (mouse), human epidemiology, or TLV.

A45 - DOSE-EFFECTS WORKSHEET

Agent Name CARBON DISULFIDE

Effect CARDIOVASCULAR DISEASE in species MAN

Dose-response relationship:



Justification: ABOUT 4% EXCESS MORTALITY WAS SEEN IN VISCOSE RAYON WORKERS EXPOSED TO 20 ppm. 1-2 ppm APPEARS TO REPRESENT A REASONABLE THRESHOLD.

---

[1] Incidence, fractional, of effect at dose shown. Enter scale as required (maximum 1.0). Excess over background is implied.

A45 - (concluded)

N_i Number at Risk[2]	C Concentration /Units	E Exposure[3] Factor/Units	D=CxE Dose /Units	D´ Converted Dose/Units	I_i Incidence	NC_i Cases
200	3.5×10^{-2} $\mu g/m^3$			.012 ppm	0	0
2×10^4	$2\text{-}1\times10^{-2}$ "			.007 "	0	0
2×10^8	6.4×10^{-4}			2×10^{-4} "	0	0
2×10^2*				.7 ppm	0	0
50				2.8 "	.001	.05
10				14 "	.025	.25
2				70 "	.12	.24
					Total Cases	.6

* SEE ATTACHED SHEET

In some cases it may be simpler to express the exposure dose information as a distribution, dN/dD (number per unit dose) as a function of D. The number of cases is then given by

$$NC = \int_{\text{Threshold}}^{\text{Saturation}} \frac{dN}{dD} (D)\ I\ (D)\ dD$$

---

[2] Absolute number or percent of total population (show with %). See also high dose distribution discussion, A45-2.

[3] See Table 45.1, BDB, Altman, Prosser, or Dill.

Carbon Disulfide--High Dose Distribution

Although the computed concentrations for CS_2 are below the threshold for cardiovascular effects even for the smallest populations, there could be hot spots that might lead to increased risk. Let us assume that the number of people exposed to higher concentrations varies inversely with the concentration, starting with the 2×10^4 concentration of .007 ppm. The results are shown in the lower part of Worksheet A45.

Aesthetics

The odor threshold for CS_2 appears to be around .025 ppm. This is only slightly higher than peak concentrations predicted on a year-round basis, so that odor episodes are likely. Let us assume that the smell becomes noticeable 10 times per year near (< 2.5 km) Claus Plants and rayon, rubber, and chemicals manufacturing. There are approximately 250 such operations. Although some will be remote, most are probably close to urbanized areas. Each might affect some 8 square miles at perhaps 200 persons/square mile, or $8 \times 200 \times 250 \times 10 = 4 \times 10^6$ instances per year. There might be additional instances associated with large stationary sources equipped with catalysts. It should be remembered that these sources are also sources of H_2S, although the latter disappears more rapidly than CS_2.

A47 - HAZARD RANKING WORKSHEET (page 1 of 1)

Agent Name CARBON DISULFIDE

1. Effect	2. Cases/ Units	3. Value	Ranking Index (2.x3.)
CARDIOVASCULAR/MAN	.6	1000	600
ODOR INCIDENTS	4×10^6	1	4×10^6

Page Total (Environmental Hazard Index) 4×10^6

Sum of 1 pages (Total Environmental Hazard Index) 4×10^6 *

Date	Rank**

---

* Applicable only to last page of multi-page forms.

** Enter new rank each time it changes as a result of new entries to the list.

TRACE OF PROCEDURE

Agent Name CARBON DISULFIDE

Branch

		AE	A, I	AD	L		
			A1-A8				
			I1-I5				
			A15-A17				
				AD1-AD3			
				AD5-AD7			
				AD9-AD1			
			A18-A19				
		AE1-AE3					
		AE7-AE8					
		AE12					
			I6				
			A20-A22				
			I7-I8				
			A23-A28				
			A31-A36		L1		
			A37-A48				
			END				

Enter step numbers encountered in ranking agent. If sequential, use nomenclature like A3-A7. Use each column for a different branch. It is often useful to place Branch A near the center.

Carbon Disulfide--Narrative

Carbon disulfide is produced in large quantities both for intermediate uses (rayon and cellophane, carbon tetrachloride, other organic chemicals) and dispersive ones (solvents, fumigants, corrosion inhibitors). It is also produced in reduction of carbonaceous sulfur, as in Claus sulfur recovery plants, and possibly in automotive catalytic converters and (in the future) stationary source converters. Most of the CS_2 will enter the air.

In the environment, CS_2 degrades to carbonyl sulfide and other products through oxidation by free oxygen atoms in the air and (possibly) photooxidation. This occurs within a few days. Even more rapid transfers occur from water and land to air, and the air is the principal reservoir.

A variety of toxic effects have been observed for CS_2 at high concentrations (> 20 ppm), but at lower ones the most prominent health effect is increased risk of cardiovascular disease. The aesthetic impacts of CS_2 may be considerable, however, because it has an unpleasant odor at very low concentrations.

If the value placed on aesthetic effects is comparable to that placed on health and ecological impacts, carbon disulfide ranks near or at the top of the candidate list. If aesthetic effects are ignored, it becomes, at best, of average concern.

Carbon Disulfide--Procedural Difficulties

Carbon disulfide presented relatively little procedural difficulty as our comprehensive study provided most of the necessary data. Difficulties occurred in:

- Not discovering the catalytic conversion source until it was pointed out after the first draft of the CS_2/COS paper.
- Needing to make a dose-distribution assumption to estimate any health effects.
- Making subjective estimates of odor instances.

Carbon Disulfide--Recommendations

Additional sensitivity studies on the value of aesthetic impacts are suggested.

Cyanides

D5 - MULTIPLE AGENTS

If Agent is represented by several compounds, list them here.

Agent as initially designated or defined CYANIDES

Representatives	Reason for Choice
HYDROGEN CYANIDE	LARGE COMMERCIAL PRODUCTION
	FATS OF CYANIDES IN ACID SOLUTIONS,
	MOST TOXIC TO FISH
POTASSIUM CYANIDE	SOURCE OF ION
SODIUM CYANIDE	LARGE COMMERCIAL PRODUCTION
	SOURCE OF ION

Preceding page blank

A2 - AGENT IDENTIFICATION

Fill in applicable sections

Agent Name HYDROGEN CYANIDE

Common Synonyms[1] HYDROCYANIC ACID
PRUSSIC ACID

☒ Chemical ☐ Physical ☐ Radiological
☐ Biological ☐ Other

For chemical agents:

☒ Compound ☐ Element ☐ Mixture

CAS Registry No.[1] 74908

Molecular Formula[1] CHN

Structural Formula[2]: $H-C\equiv N$

Melting Point[3] -13.24 °C

Boiling Point[3] 25.7 °C

Vapor Pressure[3] @20°C ~700 mmHg

Density[3] @ 20°C 0.69 Kg/l

Water Solubility,[3] 20°C ∞ Kg/l

Partition Coefficient[4] ~10:1

For physical agents:

☐ thermal ☐ particulate ☐ solid waste

Description/definition:

Temperature ______ °C (for thermal agents)

Density ______ Kg/l (for particulates)

Particle Size ______ microns (for particulates)

A2 - AGENT IDENTIFICATION

Fill in applicable sections

Agent Name POTASSIUM CYANIDE

Common Synonyms[1] HYDROCYANIC ACID, POTASSIUM SALT

☒ **Chemical** ☐ **Physical** ☐ **Radiological**

☐ **Biological** ☐ **Other**

For chemical agents:

☒ **Compound** ☐ **Element** ☐ **Mixture**

CAS Registry No.[1] 5373080; 151508

Molecular Formula[1] CNK

Structural Formula[2]: $K^{+-}C \equiv N$

Melting Point[3] 634.5 °C

Boiling Point[3] NA °C

Vapor Pressure[3] @20°C NA mmHg

Density[3] @ 20°C 1.52 Kg/l 16°C

Water Solubility,[3] 20°C .5 Kg/l 25°C

Partition Coefficient[4] NA

For physical agents:

☐ **thermal** ☐ **particulate** ☐ **solid waste** ☐ **other**

Description/definition: ______

Temperature ______ °C (for thermal agents)

Density ______ Kg/l (for particulates)

Particle Size ______ microns (for particulates)

A2 - AGENT IDENTIFICATION

Fill in applicable sections

Agent Name SODIUM CYANIDE

Common Synonyms[1] HYDROCYANIC ACID, SODIUM SALT

☒ Chemical ☐ Physical ☐ Radiological

☐ Biological ☐ Other

For chemical agents:

☒ Compound ☐ Element ☐ Mixture

CAS Registry No.[1] 14339

Molecular Formula[1] CNNa

Structural Formula[2]: $Na^{+}\,{}^{-}C \equiv N$

Melting Point[3] 563.7 °C

Boiling Point[3] 1496 °C

Vapor Pressure[3] @20°C $\ll 1$ mmHg

Density[3] @ 20°C NA Kg/l

Water Solubility,[3] 20°C .48 Kg/l 10°C

Partition Coefficient[4] NA

For physical agents:

☐ thermal ☐ particulate ☐ solid waste ☐ other

Description/definition: ________

Temperature ________ °C (for thermal agents)

Density ________ Kg/l (for particulates)

Particle Size ________ microrons (for particulates)

A4 - EFFECTS CHECKLIST

Agent Name CYANIDE

Check the suspected effects

Human: ☒ Mortality through ACUTE TOXICITY
☐ Serious disease or injury
☐ Other disease or injury
☐ Physiological effects
☐ Aesthetic impact through
☐ Economic impact through

Animal: ☒ Mortality through ACUTE TOXICITY
☐ Reproduction impairment through
☐ Yield reduction through

Plant: ☐ Mortality through
☐ Reproduction impairment through
☐ Yield reduction through

Other: ☐ Ecosystem disturbances through

Describe the principal concern: ACCIDENTAL ACUTE CN EXPOSURES BOTH TO MAN, FISH, AND RUMINANTS. THE LATTER ARE SOMETIMES EXPOSED TO NATURAL CYANIDES IN VEGETATION.

This worksheet and worksheet A2 should be reviewed with the nominator before major ranking steps are undertaken.

A20 - RELEASE WORKSHEET

Agent Name HYDROGEN CYANIDE

☒ produced commercially ☐ other human sources[1]

P	1.5 x 10^8	Kg/yr	production
I		Kg/yr	imports
E		Kg/yr	exports
IU	1.1 x 10^8	Kg/yr	intermediate uses
DU	8.6 x 10^7	Kg/yr	dispersive uses

(P + I - E - IU ☒, or directly ☐)

Releases during production (fractional)			Releases during use (fractional)	
Air	e_A	.05	f_A	1
Water	e_W	0	f_W	0
Land	e_L	.05	f_L	0

Release Rate Computation

	Production	Use	Transportation	Other	Total	
Air	$P \times e_A$ = 7.5 x 10^6	+ $DU \times f_A$ 8.6 x 10^7	+	+	= 9.4 x 10^7	Kg/yr
Water	$P \times e_W$ = 0	+ $DU \times f_W$	+	+	= 0	Kg/yr
Land	$P \times e_L$ = 7.5 x 10^6	+ $DU \times f_L$	+	+	= 7.5 x 10^6	Kg/yr

Derivation of Estimates (Document with brief narrative)

Production Processes

CATALYTIC OXIDATION OF AMMONIA METHANE MIXTURES.

---

[1] Includes combustion products, release during other activities as waste, etc. May be available in basic documents or calculable from EF.

A20 (concluded)

HYDROGEN CYANIDE

Intermediate Uses

WIDE VARIETY OF ORGANIC CHEMICALS, CYANIDE SALTS, DYES, ETC.

Dispersive Uses

FUMIGANT

Transportation Releases

Other Releases

A20 - RELEASE WORKSHEET

Agent Name SODIUM CYANIDE

☒ produced commercially ☐ other human sources[1]

P 2.1×10^7 Kg/yr production
I 5.3×10^6 Kg/yr imports
E 5.4×10^6 Kg/yr exports
IU 1.4×10^7 Kg/yr intermediate uses
DU 1.4×10^7 Kg/yr dispersive uses

(P + I - E - IU ☐, or directly ☒)

Releases during production (fractional)			Releases during use (fractional)	
Air	e_A	0	f_A	0
Water	e_W	.05	f_W	1
Land	e_L	.05	f_L	0

Release Rate Computation

	Production		Use		Transportation		Other		Total	
Air	$P \times e_A =$ 0	+	$DU \times f_A$ 0	+		+		=	0	Kg/yr
Water	$P \times e_W =$ 1.1×10^6	+	$DU \times f_W$ 1.4×10^7	+		+		=	1.5×10^7	Kg/yr
Land	$P \times e_L =$ 1.1×10^6	+	$DU \times f_L$ 0	+		+		=	1.1×10^6	Kg/yr

Derivation of Estimates (Document with brief narrative)

Production Processes

NEUTRALIZATION OF HCN BY SODIUM HYDROXIDE

---

[1] Includes combustion products, release during other activities as waste, etc. May be available in basic documents or calculable from EF.

A20 (concluded)

SODIUM CYANIDE

Intermediate Uses

ADIPONITRILE, EDTA, SODIUM FERROCYANIDE

DYES, PHARMACEUTICALS, PLASTICS, VITAMINS

Dispersive Uses

ELECTROPLATING OF COPPER, ZINC, BRASS, AND

CADMIUM; STEEL HARDENING

FROTH FLOTATION OF ORES

Transportation Releases

Other Releases

A20 - RELEASE WORKSHEET

Agent Name POTASSIUM CYANIDE

☒ produced commercially ☐ other human sources[1]

P	1×10^4	Kg/yr	production
I	9.1×10^5	Kg/yr	imports
E		Kg/yr	exports
IU	8.3×10^5	Kg/yr	intermediate uses
DU	9×10^4	Kg/yr	dispersive uses

(P + I - E - IU ☒, or directly ☐)

Releases during production (fractional)			Releases during use (fractional)	
Air	e_A	0	f_A	0
Water	e_W	0	f_W	.5
Land	e_L	.05	f_L	.5

Release Rate Computation

	Production		Use		Transportation		Other		Total	
Air	$P \times e_A =$ 0	+	$DU \times f_A$ 0	+		+		=	0	Kg/yr
Water	$P \times e_W =$ 0	+	$DU \times f_W$ 4.5×10^4	+		+		=	4.5×10^4	Kg/yr
Land	$P \times e_L =$ 5×10^2	+	$DU \times f_L$ 4.5×10^4	+		+		=	4.5×10^4	Kg/yr

Derivation of Estimates (Document with brief narrative)

Production Processes

NEUTRALIZATION OF HCN WITH POTASSIUM HYDROXIDE

---

[1] Includes combustion products, release during other activities as waste, etc. May be available in basic documents or calculable from EF.

A20 (concluded)

POTASSIUM CYANIDE

Intermediate Uses

CYANOGEN MANUFACTURE

MALONIC ACID

Dispersive Uses

ELECTROPLATING - SILVER AND COPPER

NITRIDING STEEL

Transportation Releases

Other Releases

A32 - TRANSPORT/TRANSFORMATION WORKSHEET

Agent Name HYDROGEN CYANIDE

1. Chemical Transformation (Steps A25 - A31)

Air: k_{OH} ____ $(Yr)^{-1}$/mole k_{O_3} ____ $(Yr)^{-1}$/mole T_A 1.0 Yr

Water: k_{RO_2} ____ $(Yr)^{-1}$/mole k_h ____ $(Yr)^{-1}$/mole T_W 1.0 Yr

Soil: P ____ K_e ____ T_L 1.0 Yr (ASSUMED TRANSFORMATION TO LESS TOXIC FORMS)

2. Intermedia Transfer (Step A35)

Transfer rates, in $(Yr)^{-1}$, from column heading to row heading

	Air	Water	Land
Air	—		
Water	2.3	—	1.4
Land			—

3. Steady State Inventory (Step A32)

Solve ~~[R] — [λ] [SSI]~~ equations shown in discussion LI

R_A 9.4×10^7 Kg/yr SSI_A 3.1×10^7 Kg

R_W 0 Kg/yr SSI_W 1.1×10^8 Kg

R_S 7.5×10^6 Kg/yr SSI_L 3.6×10^6 Kg

4. Non-steady State Correction (Step A33)

CF_A ____ SSI_A ____ Kg

CF_W ____ SSI_W ____ Kg

CF_L ____ SSI_L ____ Kg

5. River/Lake Partition (see discussion A39)

Lakes f .5   SSI 5.5×10^7 Kg

Rivers f .5   SSI 5.5×10^7 Kg

HYDROGEN CYANIDE

6. Concentrations (Step A39)

	Dilution Factors, D	Fraction of SSI, f_D	Concentration[1]
Air	10^6 m^3	10^{-10}	3×10^9 Kg/m^3
	10^8 m^3	10^{-8}	3×10^9 Kg/m3
	10^{10} m^3	10^{-6}	3×10^9 Kg/m^3
	10^{12} m^3	10^{-4}	3×10^9 Kg/m^3
	10^{14} m^3	10^{-2}	3×10^9 Kg/m^3
	10^{16} m^3	.99	3×10^9 Kg/m^3
Rivers	10^{11} 1	10^{-4}	5×10^{-8} Kg/1
	10^{12} 1	9×10^{-4}	5×10^{-8} Kg/1
	10^{13} 1	9×10^{-3}	5×10^{-8} Kg/1
	10^{14} 1	9×10^{-2}	5×10^{-8} Kg/1
	10^{15} 1	9×10^{-1}	5×10^{-8} Kg/1
Lakes	3×10^6 1	3×10^{-9}	5.5×10^{-8} Kg/1
	3×10^8 1	3×10^{-7}	5.5×10^{-8} Kg/1
	3×10^{10} 1	2×10^{-5}	3.6×10^{-8} Kg/1
	3×10^{12} 1	2×10^{-3}	3.6×10^{-8} Kg/1
	3×10^{14} 1	2×10^{-2}	3.6×10^{-9} Kg/1
	3×10^{16} 1	.98	1.8×10^{-9} Kg/1
Land	5×10^6 m^2		Kg/m^2
	5×10^8 m^2		Kg/m^2
	5×10^{10} m^2		Kg/m^2
	5×10^{12} m^2		Kg/m^2

---

[1] If release rate and/or transformation rate data are inadequate, use ambient concentrations observed, from SAROAD and STORET.

A32 - TRANSPORT/TRANSFORMATION WORKSHEET

Agent Name POTASSIUM AND SODIUM CYANIDE

1. Chemical Transformation (Steps A25 - A31)

Air: K_{OH} ____ $(Yr)^{-1}$/mole K_{O_3} ____ $(Yr)^{-1}$/mole T_A 1 Yr

Water: K_{RO_2} ____ $(Yr)^{-1}$/mole K_1 ____ $(Yr)^{-1}$/mole T_W 1 Yr

Soil: P ____ K_e ____ T_L 1 Yr

2. Intermedia Transfer (Step A35)

Transfer rates, in $(Yr)^{-1}$, from column heading to row heading

	Air	Water	Land
Air	—		
Water		—	1.4
Land			—

3. Steady State Inventory (Step A32)

Solve ~~{R} = {λ} {SSI}~~ equations shown in discussion LI

R_A 0 Kg/yr SSI_A 0 Kg

R_W 1.5×10^7 Kg/yr SSI_W 2.3×10^7 Kg

R_S 1.1×10^6 Kg/yr SSI_L 5×10^5 Kg

4. Non-steady State Correction (Step A33)

CF_A ____ SSI_A ____ Kg

CF_W ____ SSI_W ____ Kg

CF_L ____ SSI_L ____ Kg

5. River/Lake Partition (see discussion A39)

Lakes f .5 SSI 1.1×10^7 Kg

Rivers f .5 SSI 1.1×10^7 Kg

POTASSIUM AND SODIUM CYANIDE

6. Concentrations (Step A39)

	Dilution Factors, D	Fraction of SSI, f_D	Concentration[1]
Air	10^6 m^3		Kg/m^3
	10^8 m^3		Kg/m3
	10^{10} m^3		Kg/m^3
	10^{12} m^3		Kg/m^3
	10^{14} m^3		Kg/m^3
	10^{16} m^3		Kg/m^3
Rivers	10^{11} l	10^{-4}	1.1×10^{-8} Kg/l
	10^{12} l	9×10^{-4}	1.0×10^{-8} Kg/l
	10^{13} l	9×10^{-3}	1.0×10^{-8} Kg/l
	10^{14} l	9×10^{-2}	1.0×10^{-8} Kg/l
	10^{15} l	9×10^{-1}	1.0×10^{-8} Kg/l
Lakes	3×10^6 l	3×10^{-9}	1.1×10^{-8} Kg/l
	3×10^8 l	3×10^{-7}	1.1×10^{-8} Kg/l
	3×10^{10} l	2×10^{-5}	7×10^{-9} Kg/l
	3×10^{12} l	2×10^{-3}	7×10^{-9} Kg/l
	3×10^{14} l	2×10^{-2}	7×10^{-10} Kg/l
	3×10^{16} l	.98	3.6×10^{-10} Kg/l
Land	5× 5×10^6 m^2 *	1% GRASS	2×10^{-4} Kg/m^2
	5×10^8 m^2		Kg/m^2
	5×10^{10} m^2		Kg/m^2
	5×10^{12} m^2		Kg/m^2

---

[1] If release rate and/or transformation rate data are inadequate, use ambient concentrations observed, from SAROAD and STORET.

* ASSUMED LAND DISPOSAL REACHING PASTURES

A41 - BIOLOGICAL EFFECTS CHECKLIST

Agent Name CYANIDES

Species at risk: (select no more than 5)

☒ Man
☒ Domestic animals SHEEP
☐
☒ Other animals FISH
☐
☐
☐ Crops
☐
☐
☐ Other plants
☐
☐

Effects to be considered: (select[1] no more than 3 for men, 1 each for other species)

Species	Effects	Indicator Test[2]
Man	ACUTE TOXICITY	CASE HISTORIES
SHEEP	ACUTE TOXICITY	EXPERIMENT
FISH	ACUTE TOXICITY	EXPERIMENT

---

[1] Selection should be based on suspected dominance of value once ranking is complete.

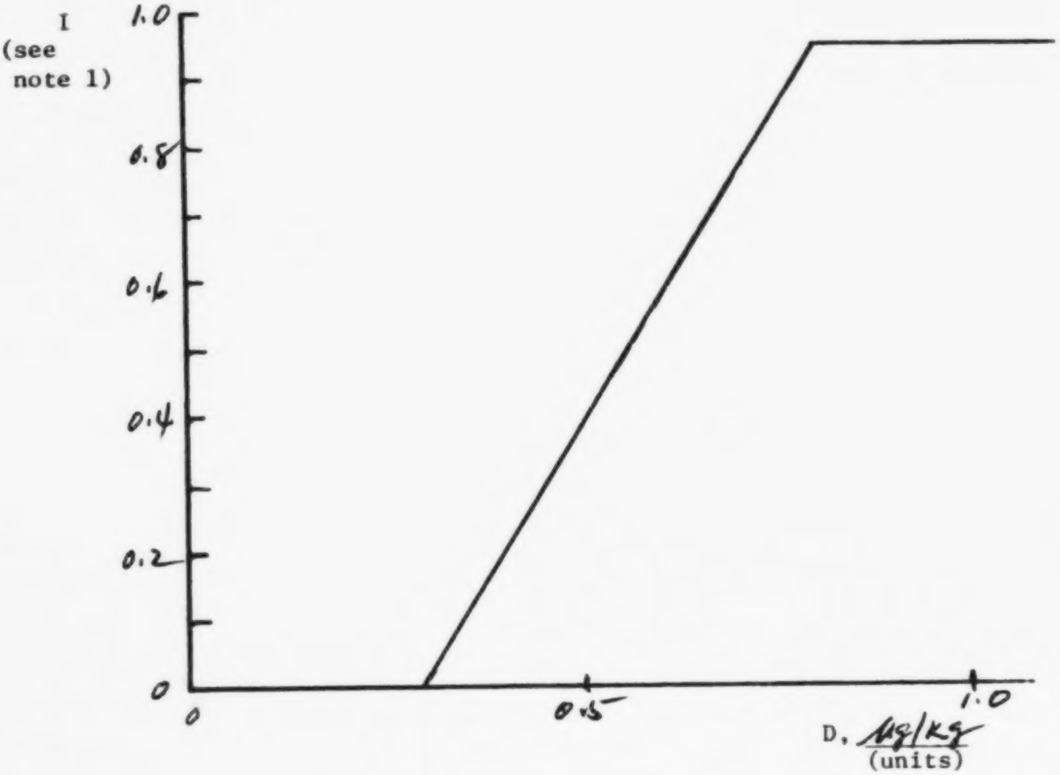
[2] For example, LD_{50} (mouse), human epidemiology, or TLV.

A45 - DOSE-EFFECTS WORKSHEET

Agent Name HYDROGEN CYANIDE

Effect ACUTE TOXICITY in species MAN

Dose-response relationship:



Justification: THRESHOLD LEVELS FOR CYANIDE POISONING ARE PRETTY WELL KNOWN FROM CASE HISTORIES. SUBACUTE DOSES SEEM TO HAVE NO LASTING EFFECTS

---

[1] Incidence, fractional, of effect at dose shown. Enter scale as required (maximum 1.0). Excess over background is implied.

HYDROGEN CYANIDE

AA5 - (Concluded)

N Number at Risk[2]	C Concentration /Units	E Exposure[3] Factor/Units	D=CxE Dose /Units	D' Converted Dose/Units	I_i Incidence	NC_i Cases
$1 x 10^8$	$5.5 x 10^{-2}$ µg/l	1.5 l/day	$8 x 10^{-2}$ µg/day		0	0
10^8*			.1 µg/kg		0	0
$6 x 10^3$			.4 "		.2	1200
$4 x 10^3$			.5 "		.4	1600
$3 x 10^3$			.6 "		.6	1800
$2 x 10^3$			.7 "		.8	1600
					Total Cases	6000

* SEE ATTACHED SHEET

In some cases it may be simpler to express the exposure dose information as a distribution, dN/dD (number per unit dose) as a function of D. The number of cases is then given by

$$NC = \int_{\text{Threshold}}^{\text{Saturation}} \frac{dN}{dD}(D)\, I\,(D)\, dD$$

---

[2] Absolute number or percent of total population (show with %). See also high dose distribution discussion, AA5.2.

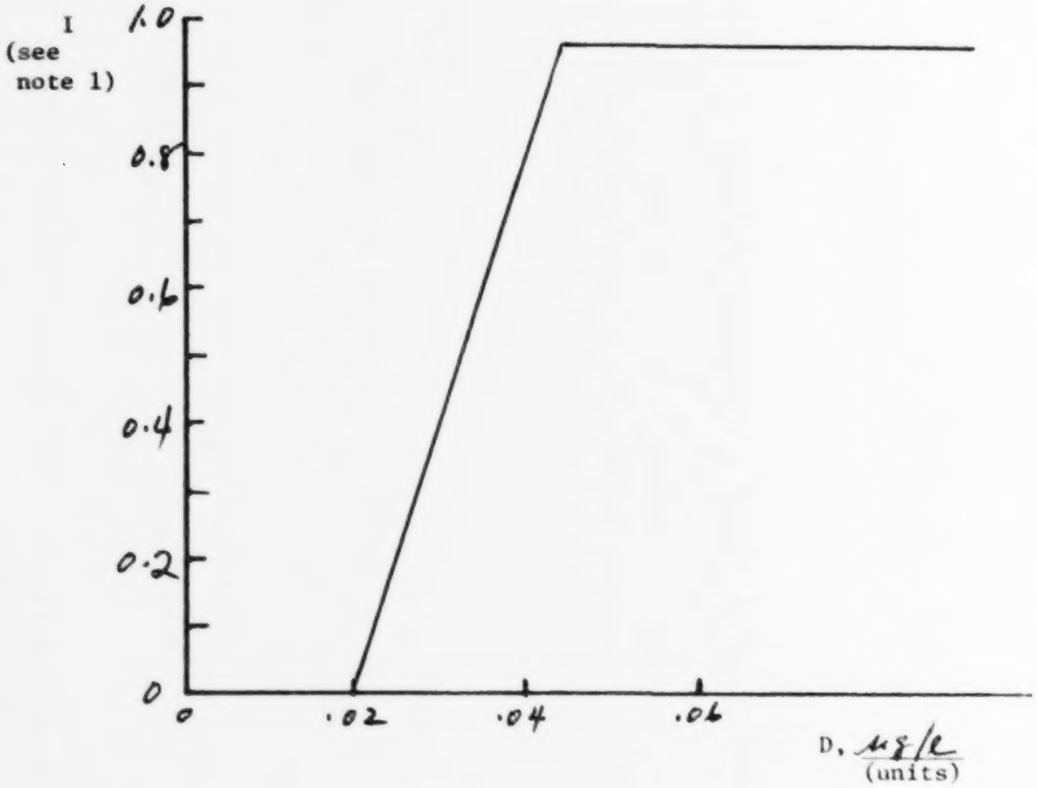
[3] See Table A5.1, EDR, Altman, Prosser, or DOII.

A45 - DOSE-EFFECTS WORKSHEET

Agent Name CYANIDE ION

Effect ACUTE TOXICITY in species TROUT

Dose-response relationship:



Justification: TROUT IS AN EXAMPLE OF A SPECIES SENSITIVE TO CYANIDES

---

1 Incidence, fractional, of effect at dose shown. Enter scale as required (maximum 1.0). Excess over background is implied.

CYANIDE ION

A45 - (concluded)

N_i Number at Risk[2]	C Concentration /Units	E Exposure[3] Factor/Units	D=CxE Dose /Units	D´ Converted Dose/Units	I_i Incidence	NC_i Cases
100 %	1.0×10^{-2} µg/l		1.0×10^{-2} µg/l		0	0
25 %*			2×10^{-2} µg/l		0	0
11 %			3×10^{-2} 〃		.4	4.4%
6 %			4×10^{-2} 〃		.7	4.2%
4 %			5×10^{-2} 〃		1.0	4.0%

*SEE ATTACHED SHEET

Total Cases 13%

In some cases it may be simpler to express the exposure dose information as a distribution, dN/dD (number per unit dose) as a function of D. The number of cases is then given by

$$NC = \int_{\text{Threshold}}^{\text{Saturation}} \frac{dN}{dD}(D)\ I\ (D)\ dD$$

---

[2] Absolute number or percent of total population (show with %). See also high dose distribution discussion, A45.2.

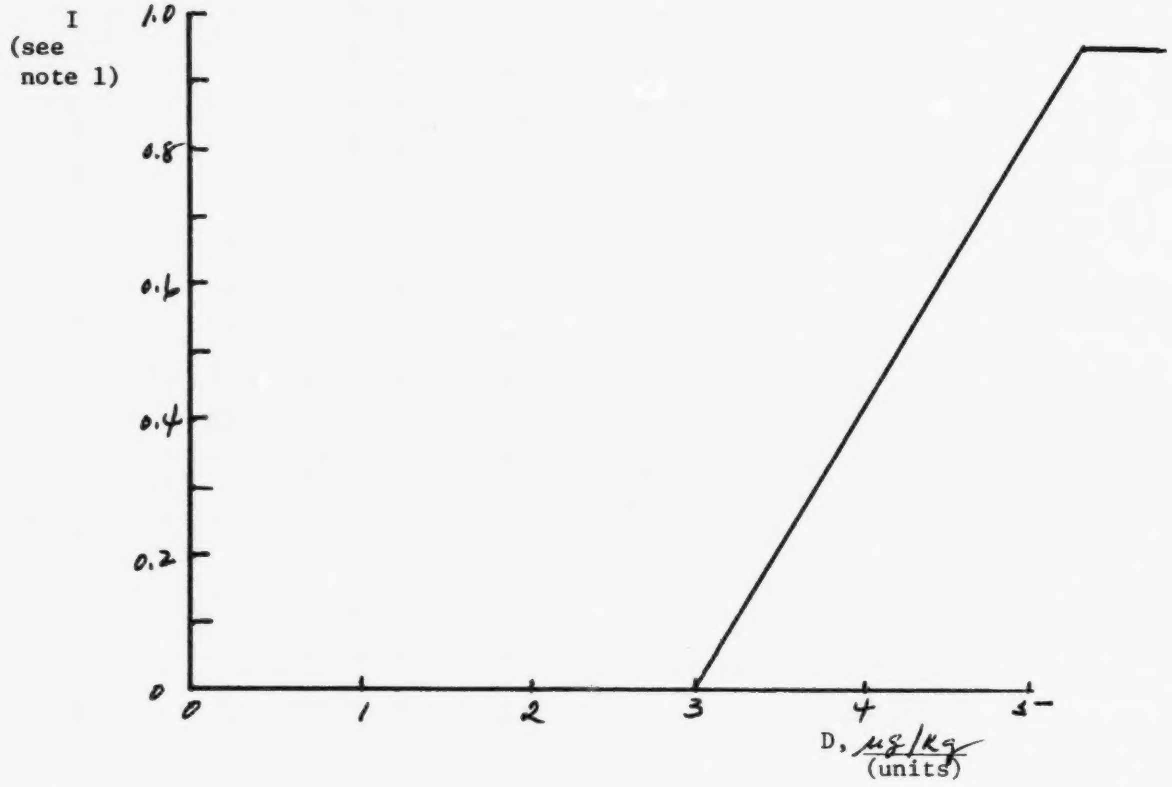
[3] See Table 45.1, BDB, Altman, Prosser, or Dill.

A45 - DOSE-EFFECTS WORKSHEET

Agent Name CYANIDE ION

Effect ACUTE TOXICITY in species SHEEP

Dose-response relationship:



Justification: EXPERIMENTAL RESULTS

---

[1] Incidence, fractional, of effect at dose shown. Enter scale as required (maximum 1.0). Excess over background is implied.

CYANIDE ION

A45 - (concluded)

N_i Number at Risk[2]	C Concentration /Units	E Exposure[3] Factor/Units	D=CxE Dose /Units	D´ Converted Dose/Units	I_i Incidence	NC_i Cases
130*	200 μg/m^2	30 m^2/DAY	6×10^3 μg/DAY	100 μg/kg	1.0	130

*ASSUMED GRAZING ON THE CONTAMINATED GRASS

Total Cases 130

≈ .013%

In some cases it may be simpler to express the exposure dose information as a distribution, dN/dD (number per unit dose) as a function of D. The number of cases is then given by

$$NC = \int_{\text{Threshold}}^{\text{Saturation}} \frac{dN}{dD}(D)\ I\ (D)\ dD$$

---

[2] Absolute number or percent of total population (show with %). See also high dose distribution discussion, A45.2.

[3] See Table 45.1, BDB, Altman, Prosser, or Dill.

Cyanide ion--High Dose Distribution

The predicted levels are dangerously close to lethal. Let us assume that the population exposed to higher levels varies inversely with the concentration squared. The results are shown in the lower part of Worksheet A45.

Hydrogen Cyanide--High Dose Distribution

The average dose of cyanides is well below the threshold. However, in the real world, concentrations could accidentally rise above this level. Let us assume that the number of people exposed to larger concentrations varies inversely with dose squared. The results are shown in the lower part of the A45 worksheet.

A47 - HAZARD RANKING WORKSHEET (page 1 of 2)

Agent Name HYDROGEN CYANIDE

1. Effect	2. Cases/ Units	3. Value	Ranking Index (2.x3.)
ACUTE TOXICITY/MAN	6000	1000	6×10^6

Page Total (Environmental Hazard Index) 6×10^6

Sum of 1 pages (Total Environmental Hazard Index) ______*

Date	Rank**

---

* Applicable only to last page of multi-page forms.

** Enter new rank each time it changes as a result of new entries to the list.

A47 - HAZARD RANKING WORKSHEET (page 2 of 2)

Agent Name CYANIDE ION

1. Effect	2. Cases/ Units	3. Value	Ranking Index (2.x3.)
ACTUTE TOXICITY/SHEEP	.013%	10,000/%	130
ACUTE TOXICITY/TROUT	13 %	1000/%	13,000

Page Total (Environmental Hazard Index) 13,000

Sum of 2 pages (Total Environmental Hazard Index) 6×10^6 *

Date	Rank**

---

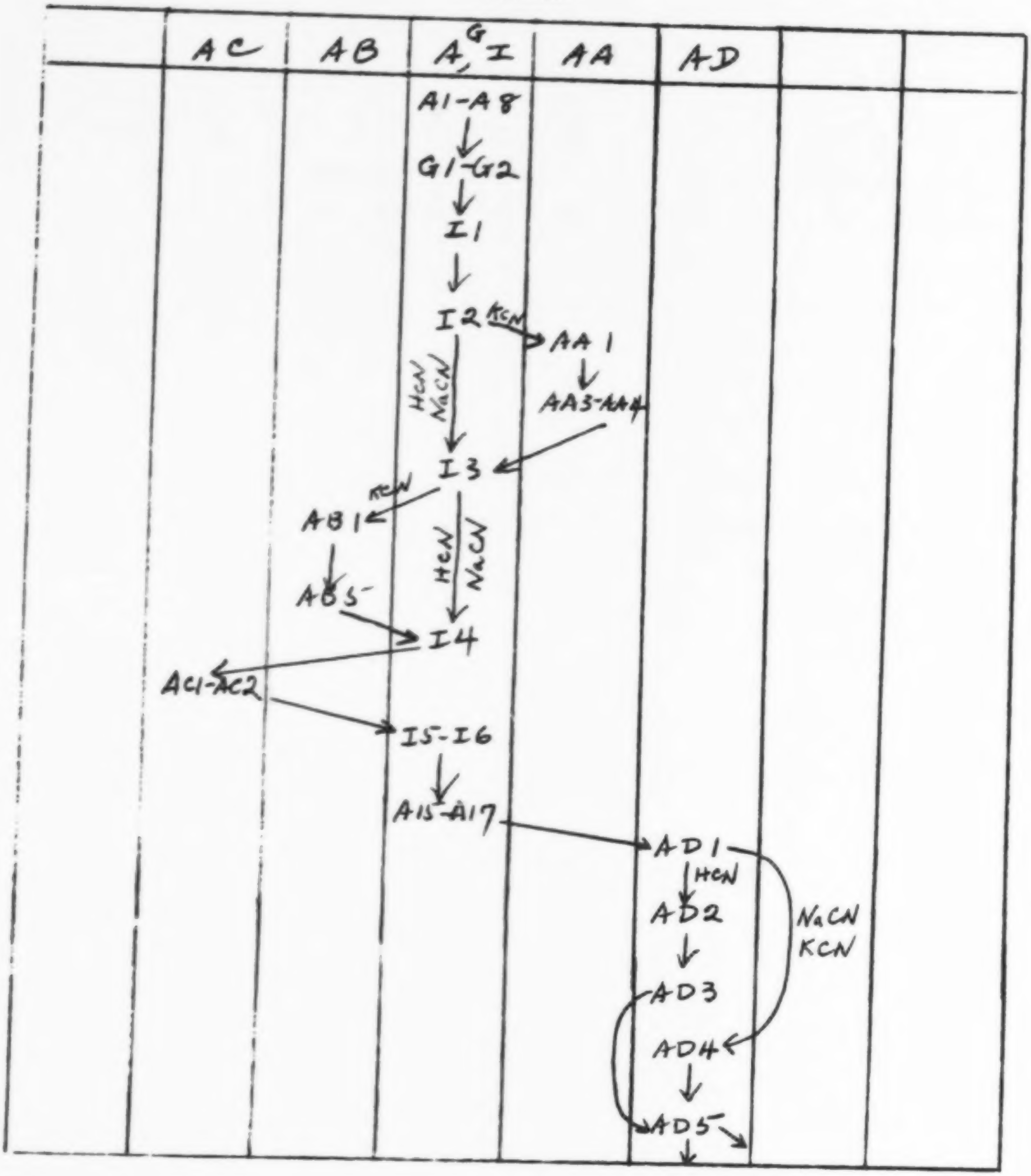
* Applicable only to last page of multi-page forms.

** Enter new rank each time it changes as a result of new entries to the list.

TRACE OF PROCEDURE

Agent Name CYANIDES

Branch

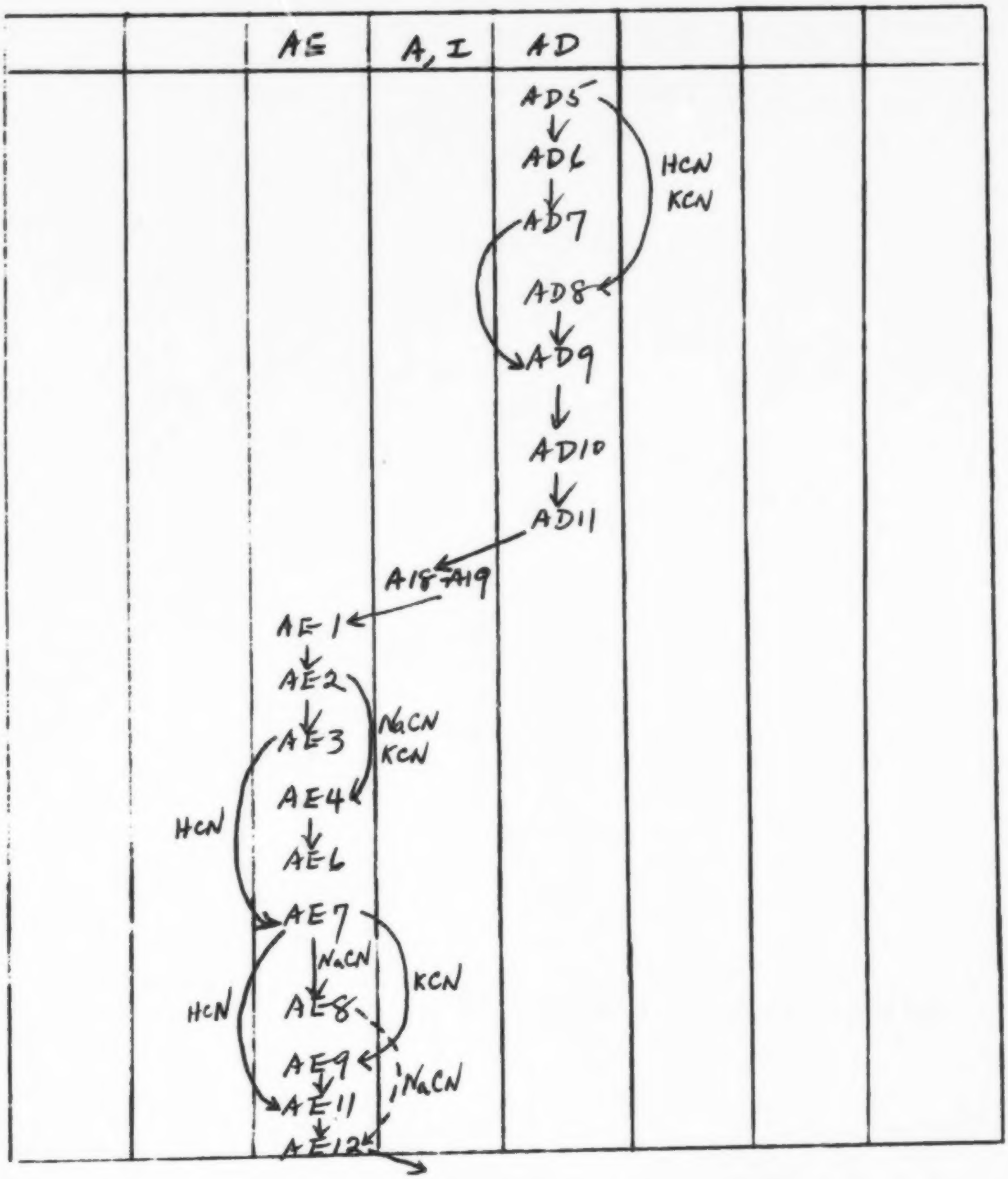

AC
AB
A, G, I
AA
AD
A1-A8
G1-G2
I1
I2
KCN
AA1
HCN
NaCN
AA3-AA4
I3
KCN
AB1
HCN
NaCN
AB5
I4
AC1-AC2
I5-I6
A15-A17
AD1
HCN
AD2
NaCN
KCN
AD3
AD4
AD5

Enter step numbers encountered in ranking agent. If sequential, use nomenclature like A3-A7. Use each column for a different branch. It is often useful to place Branch A near the center.

TRACE OF PROCEDURE

Agent Name CYANIDES 2

Branch

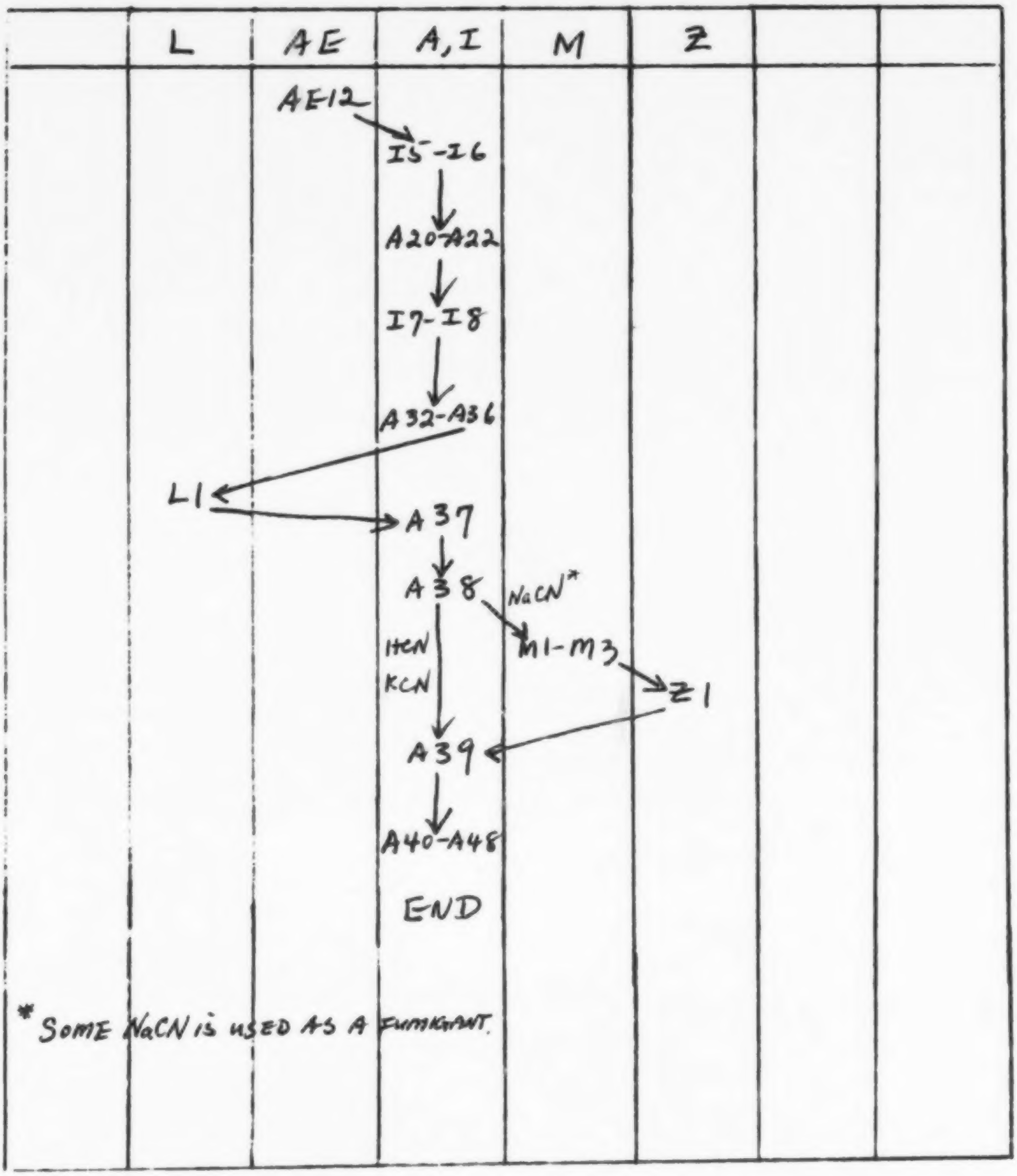

AE
A, I
AD
AD5
AD6
AD7
HCN
KCN
AD8
AD9
AD10
AD11
A18-A19
AE1
AE2
AE3
NaCN
KCN
AE4
HCN
AE6
AE7
NaCN
KCN
HCN
AE8
AE9
NaCN
AE11
AE12

Enter step numbers encountered in ranking agent. If sequential, use nomenclature like A3-A7. Use each column for a different Branch. It is often useful to place Branch A near the center.

TRACE OF PROCEDURE

Agent Name CYANIDES 3

Branch


L
AE
A, I
M
Z
AE12
I5-I6
A20-A22
I7-I8
A32-A36
L1
A37
A38
NaCN*
HCN
KCN
M1-M3
Z1
A39
A40-A48
END

*SOME NaCN IS USED AS A FUMIGANT.

Enter step numbers encountered in ranking agent. If sequential, use nomenclature like A3-A7. Use each column for a different branch. It is often useful to place Branch A near the center.

Cyanides--Narrative

Cyanides were represented by the precursor (and sometimes end product) hydrogen cyanide and two salts, sodium and potassium. The acid is used as a fumigant, but much more heavily as an intermediate to organic chemicals, dyes, and so on. The salts are used extensively in electroplating and steel treatment, in addition to intermediate uses for organic chemicals. The acid is assumed released to air and land, the salts to water and land.

Once in the general environment, the cyanides tend to move to the water medium (rivers and lakes assumed equal). In all media, they are assumed to react slowly (1 yr) to less toxic forms (complexes, and so on).

The cyanides are acutely toxic if the concentration is sufficiently high, but slightly lower chronic doses seem to lead only to fatigue and weakness. Toxicities to man from drinking water, to trout from river water, and to sheep from land-contaminated forage were examined. The human risk is potentially of most concern, but average doses were below threshold. Under certain conditions, cyanide deaths could be quite high. The hazard to trout is much more likely than hazard for humans.

Cyanides seem to pose a moderate to very high hazard relative to the other candidate agents.

Cyanides--Procedural Difficulties

Cyanides did not pose any unusual procedural difficulties except in the attempt to treat accidentally high dosages in man. The environmental hazard index for this effect could be as high as 10^7, but probably is much smaller (10^4 ?).

Cyanides--Recommendations

Alternative distribution models for cyanides should be tested to determine whether the high dose distribution is reasonable.

Appendix H

ABBREVIATIONS

	Abbreviations	Reference, If Applicable
ACS	American Chemical Society	American Chemical Society, 1968
BA	Biological Abstracts	*
BDB	Biology Data Book	Altman, 1974
BOD_5	Five Day Biochemical Oxygen Demand	Sawyer, 1971
CA	Chemical Abstracts	*
CAS	Chemical Abstracts Service	
CBAC	Chemical Biological Activity Catalog	
CEH	Chemical Economics Handbook	SRIa
Census	Census of Manufactures	Bureau of the Census, 1972
CHEMLINE	Chemline	**
CMR	Chemical Marketing Reporter	***
COD	Chemical Oxygen Demand	Sawyer, 1971
COM	Chemical Origins and Markets	SRIb
CPSC	Consumer Product Safety Commission	
CR	Chemical Reviews	Leo, 1971
CTCP	Clinical Toxicology of Commercial Products	Gleason, 1969
DCP	Directory of Chemical Producers	SRI, 1974
Dill	Handbook of Physiology	Dill, 1964
DOT	Department of Transportation	
Doyle	G. J. Doyle, *et al*	Doyle, 1975
EB	Environmental Biology	Altman, 1966
EEC	European Economic Community	****
EF	Emission Factors for Trace Substances	Anderson, 1973
EMIC	Environmental Mutagen Information Center	**
EPA-OAWM	Environmental Protection Agency, Office of Air and Waste Management	
EPA-OEGC	EPA, Office of Enforcement and General Council	
EPA-OHM	EPA, Office of Hazardous Materials	
EPA-OPP	EPA, Office of Pesticide Programs	
EPA-OSWMP	EPA, Office of Solid Waste Management Programs	
EPA-OTS	EPA, Office of Toxic Substances	
EPA-OWHM	EPA, Office of Water and Hazardous Materials	
FCH	Farm Chemicals Handbook	Berg, 1975
FDA	Food and Drug Administration	
FPG	Fire Protection Guide on Hazardous Materials	NFPA, 1975
FT-246	Federal Trade Commission	FTC, 1973b

Preceding page blank

	Abbreviations	Reference, If Applicable
FT-410	Federal Trade Commission	FTC, 1973a
HBT	Handbook of Toxicology	Spector, 1956
Hendry	Journal of Physical Chemistry Reference Data	Hendry, 1974
HCP	Handbook of Chemistry and Physics	Weast, 1975
IBCP	Imports of Benzenoid Chemicals and Products	ITC, 1976
IM	Index Medicus	*
JWPCF	Journal of the Water Pollution Control Federation	***
Lambert	Sorption in Soil	Lambert, 1967
Lange	Lange's Handbook of Chemistry	Dean, 1973
LC50	Concentration Lethal to 50% of Exposed Population	NIOSH, 1974
LD50	Dose Lethal to 50% of Exposed Population	NIOSH, 1974
LDLO	Lowest dose reported as lethal	NIOSH, 1974
LRPS	Long Range Planning Service	SRIc
MERCK	MERCK INDEX	Steiber, 1968
Miller	Models of Radionuclides	Miller, 1963
MP	Metabolism of Pesticides	Monzie, 1969
MY	Minerals Yearbook	Bureau of Mines
NA	Not Applicable	
NCI	National Cancer Institute File	National Cancer Institute
NEDS	National Emissions Data System	****
NIOSH	National Institute for Occupational Safety and Health	
NLM	National Library of Medicine	
NSF	National Science Foundation Study	SRI, 1975
OSHA	Occupational Safety and Health Administration	
PHS 149	Survey of Compounds Which Have Been Tested for Carcinogenic Activity	Shubik
Prosser	Comparative Animal Physiology	Prosser, 1973
SAROAD	Storage and Retrieval of Aerometric Data	****
Shepard	Catalog of Teratogenic Agents	Shepard, 1973
SOC	Synthetic Organic Chemicals	ITC, 1973
SOCMA	SOCMA Handbook	Synthetic Organic Chemical Manufacturer's Association, 1966
STORET	Storage and Retrieval of Water Data	****
Sax	Dangerous Properties or Industrial Materials	Sax, 1975
TADS	Technical Assistance Data System	****

	Abbreviations	Reference, If Applicable
TDB	Toxicology Data Bank	****
TLV	Threshold Limit Value	ACGIH, 1971
TMIC	Toxic Materials Information Center	**
TOXLINE	TOXLINE	**
TSL	Toxic Substances List	NIOSH, 1974
USCG	U.S. Coast Guard	
USDA-MID	U.S. Department of Agriculture, Meat Inspection Division	
Wilson	Journal of Chemical and Physical Reference Data	Wilson, 1972
WPPMP	Water Pollution Potential of Manufactured Products	Berkowitz, 1973
WQC	Water Quality Criteria	EPA, 1972

---

[*] See Abstracting Services in References.

[**] See Computer-Based Literature Search Services in References.

[***] See Periodicals in References.

[****] See Computer-Based Data Files in References.

Appendix I

REFERENCES

Preceding page blank

REFERENCES

Altman, P. L. and D. S. Dittmer, ed., Environmental Biology, Fed. Amer. Soc. Expt. Biol., Bethesda, Maryland. 694 p. (1966).

Altman, P. L. and D. S. Dittmer, ed., Biology Data Book, 2nd ed. Fed. Amer. Soc. Expt. Biol., Bethesda, Maryland. 2123 p. (1974).

American Chemical Society, Oxidation of Organic Compounds--III, Advances in Chemistry Series, 77 (1968).

American Conference of Governmental Industrial Hygienists, 1971. Documentation of the Threshold Limit Values for Substances in Workroom Air, 3rd Edition (1971).

Anderson, D., "Emission Factors for Trace Substances," EPA Report No. PB-230-894 (1973).

Anonymous, "Hot Market for Antimony Oxide," Chem. Wk., 113:21-22 (1973).

Battelle Memorial Institute, "Identification Systems for Selecting Chemical Classes as Candidates for Evaluation," EPA-5611-74001 (November 1974).

Behrens, R. G. and G. M. Rosenblatt, "Vapor Pressure and Thermodynamics of Orthorhombic Antimony Trioxide (Valentinite)," J. Chem. Thermodynamics, 5:173-188 (1973).

Berg, G. L., ed., Farm Chemicals Handbook, Meister Publishing Co. (1975).

Berkowitz, J. B., G. R. Schimke, and J. R. Valeri, "Water Pollution Potential of Manufactured Products," 4 vols. Off. of Res. & Monitoring, Environmental Protection Agency, EPA-R2-73-179A-D (1973).

Biers, W. D., "Characterization of Claus Plant Emissions," EPA Report No. EPA-72-73-188 (1973).

Boland, L. F., "Beryllium: Present and Potential Uses," The Analysts Journal, p. 27-31 (1958).

Preceding page blank

Brush Beryllium Company, "Literature on Industrial Hygiene Practices for the Control of Air-Borne Beryllium," Mimeographed Notes (1956).

Bureau of the Census, Census of Manufactures (several series) (1972).

Bureau of Mines, "Mineral Industry Surveys: Beryllium in 1974" (December 1974).

Capener, E. R. M. Wright, and S. L. Brown, Handbook of Hazardous Wastes, Federal Ministry of Interior (Germany) (1974).

Centre D/Information du Cobalt, Cobalt Monograph (Brussels) (1960).

Dean, J. A., ed., Lange's Handbook of Chemistry, 11th ed. (McGraw-Hill Book Company, New York, New York, 1973).

Dill, D. B., E. F. Adolph, and C. C. Wilber, ed., Handbook of Physiology: Section 4, Adaptation to the Environment. Amer. Physiol. Soc., Washington, D.C. 1056 p. (1964).

Doyle, G. J., A. C. Lloyd, K. R. Darnall, A. M. Winder, and J. N. Pitts, Jr., "Gas Phase Kinetic Study of Relative Rates of Reaction of Selected Aromatic Compounds with Hydroxyl Radicals in an Environmental Chamber," Environ. Sci. Tech., 9 (3) 237 (1975).

Dreisbach, R. H., Handbook of Poisoning: Diagnosis and Treatment, 5th Edition, Lange Medical Publications, Los Altos, California (1966).

Durocher, N. L., "Preliminary Air Pollution Survey of Beryllium and Its Compounds: A Literature Review," Litton Systems, Inc., Final Report, HEW Contract No. Ph 22-68-25 (1969).

Edinger, J. E., "Vertical Temperature Structure and Water Surface Heat Exchange," Water Resources Research, 6:1392-1395 (1970).

Edinger, J. E., D. W. Duttweiler, and J. C. Geyer, "The Response of Water Temperatures to Meteorological Conditions," Water Resources Research, 4:1137-1143 (1968).

Environmental Protection Agency, "Water Quality Criteria 1972," EPA-R-73-033 (March 1972).

Environmental Protection Agency. 1973a, "National Emissions Inventory of Sources and Emissions of Molybdenum," EPA-4501-3-74-009 (May 1973).

Environmental Protection Agency, 1973b, "Plutonium: Statement of the Problem," Office of Radiation Programs (mimeo), 73 p. (1973).

Environmental Protection Agency, "Proceedings of Public Hearings: Plutonium and the Other Transuranium Elements," Office of Radiation Programs, ORP/CSD-75-1 (1974).

Exxon Research and Engineering Co., "Evaluation of Pollution Control in Fossil Fuel Conversion Processes--Liquefaction: Section 2, SRC process," EPA Report No. EPA-650/2-74-009-f (1975).

Federal Trade Commission, 1973a, "U.S. Foreign Trade, Exports, Commodity by Country" (FT-410), Federal Trade Commission (1973).

Federal Trade Commission, 1973b, "U.S. Imports, General and Consumption, Schedule A, Commodity and Country" (FT-246), Federal Trade Commission, (1973).

Firm, R. J., "The Chemistry of Carbonyl Sulfide," Chem. Rev., 57:621-640 (1957).

Fishbein, L., "Environmental Health Aspects of Selenium, Tellurium and Molybdenum: A Preliminary Review, #3-Molybdenum," World Health Organization. Environmental Health Criteria Programme, Document EHE/EHC/WP/74.3 (1974).

Gleason, M. N., R. E. Gosselin, H. C. Hodge, and R. P. Smith, "Clinical Toxicology of Commercial Products," Williams & Wilkins (1969).

Goodman, L. S. and A. Gilman, The Pharmacological Basis of Therapeutics, 4th ed., The Macmillan Co., London (1970).

Hamilton, A. and H. L. Hardy, Industrial Toxicology, 3rd ed., Publishing Sciences Group, Inc., Acton, Massachusetts (1974).

Hendry, D. G., T. Mill, L. Piskiewicz, J. A. Howard, and H. K. Eigenmann, "A Critical Review of H-Atom Transfer in the Liquid Phase: Chlorine Atom, Alkyl, Trichloromethyl, Alkoxy and Alkylperoxy Radicals," J. Phys. Chem., Ref. Data, 3, 937 (1974).

Howard, P. H., "Establishing Environmental Priorities for Synthetic Organic Chemicals: Focusing on the Next PCB's from Seminar on Early Warning Systems for Toxic Substances," (February 1974).

IARC, International Agency for Research on Cancer Monograph on the Evaluation of Carcinogenic Risk of Chemicals to Man, Vol. 1:17-28 (1972).

International Trade Commission, *Synthetic Organic Chemicals* (1973).

International Trade Commission, "Imports of Benzenoid Chemicals and Products, 1974," Publication 762 (March 1976).

Jordan, T. E., *Vapor Pressures of Organic Compounds*, Interscience (New York, 1954).

Kirk-Othmer, *Encyclopedia of Chemical Technology*, 2nd ed., Wiley (1963).

Kontsoukos, E. P., J. L. Blumenthal, M. Ghassemi, and G. Baverie, "Assessment of Catalysts for Control of NO from Stationary Power Plants," EPA Report No. EPA-650/2-75-001a (1972).

Lambert, S. M., "Functional Relationship between Sorption in Soil and Chemical Structure," *J. Agr. Food Chem.*, *15* (4) 572 (1967).

Leo, A., C. Hansch and D. Elkins, "Partition Coefficients and Their Uses," *Chem. Reviews*, *71* (6) 525 (1971).

Mackay, D. and A. W. Wolkoff, "Rate of Evaporation of Low Solubility Contaminants from Water Bodies to Atmosphere," *Environ. Sci. Tech.*, *7* (7) 611 (1973).

Matheson Company, Inc., "Carbonyl Sulfide," pp. 97-100, In *Matheson Gas Data Book*, 4th ed., East Rutherford, N. J. (1966).

Miller, C. F. and S. L. Brown, "Models for Estimating the Absorbed Dose from Assimilation of Radionuclides in Body Organs of Humans," SRI Project IMU-4021 (May 1963).

Mines, Bureau of, *Minerals Yearbook*, latest edition.

Monzie, C. M., *Metabolism of Pesticides*, Wildlife No. 127, Bureau of Sports Fisheries and Wildlife (1969).

Myers, D. R., "Airborne Thermal Imagery of Discharge Plume Dispersion--Pilgrim Station," Research Report, Coastal Research Corporation (1971).

National Academy of Sciences, "Water Quality Criteria, 1972," EPA Ecological Research Series, EPA-R3-73-033, 594 p. (1972).

National Academy of Sciences, 1975a, *Assessing Potential Ocean Pollutants* (1975).

National Academy of Sciences, 1975b, Principles for Evaluating Chemicals in the Environment (1975).

National Fire Protection Association, "Fire Protection Guide on Hazardous Materials" (1975).

National Institute for Occupational Safety and Health, The Toxic Substances List (June 1974).

Novotny, V., P. A. Krenkel, "Simplified Mathematical Model of Temperature Changes in Rivers," Journal of the Water Pollution Control Federation, 45:240-248 (1973).

Peyton, T. O., R. V. Steele, and W. R. Mabey, "Carbon Disulfide, Carbonyl Sulfide: Literature Review and Environmental Assessment," Stanford Research Institute (January 1976).

Prosser, C. L., Comparative Animal Physiology, 3rd ed., W.B. Saunders Co., Philadelphia, Pa. (1966).

Reeves, A. L., D. Deitch, and A. J. Vorwald, "Beryllium Carcinogenesis. I. Inhalation Exposure of Rats to Beryllium Sulfate Aerosol," Cancer Research, 27:439.

Sawyer, C. N., and P. L. McCarty, Chemistry for Sanitary Engineers (1971).

Sax, N., Dangerous Properties of Industrial Materials, 4th ed., Van Nostrand (1975).

Shepard, T. H., Catalog of Teratogenic Agents, Johns Hopkins (1973).

Shubik, P. and J. L. Hartwell, Survey of Compounds Which Have Been Tested for Carcinogenic Activity, HEW/PHS, several volumes (1940-1973).

Spector, W. S., Handbook of Toxicology, Vol. 1, Saunders (1956).

Stanford Research Institute, a, "Chemical Economics Handbook Program," a continuing marketing research service.

Stanford Research Institute, b, Chemical Origins and Markets, "Chemical Information Services," Stanford Research Institute.

Stanford Research Institute, c, "Long Range Planning Service," a continuing service to industry.

Stanford Research Institute, Directory of Chemical Producers, an annual publication (1974).

Stanford Research Institute, "Research Program on Hazard Priority Ranking of Manufactured Chemicals," Report by Stanford Research Institute to the National Science Foundation (April 1975).

Startton, W. R., ed., Plutonium Information Meeting for an Ad Hoc Subcommittee of the Advisory Committee on Reactor Safeguards, U.S. Atomic Energy Commission, Conf-740115 (1974).

Steiber, P. G., ed., The Merck Index, 8th ed., Merck and Co., Rahway, N.J. (1968).

Stokinger, H. E., ed., Beryllium: Its Industrial Hygiene Aspects, Academic Press, N.Y. (1966).

Sundrom, T. R. and R. G. Rehn, "The Seasonal Thermal Structure of Deep Temperate Lakes," Tellus, 25:157-167 (1973).

Synthetic Organic Chemical Manufacturers' Association, SOCMA Handbook (1966).

Teisinger, J., "1972 Yant Memorial Lecture--New Advances in Toxicology of Carbon Disulfide," American Industrial Hygiene Association Journal, 35:55-61 (1974).

Timmermans, J., Physico-Chemical Constants of Pure Organic Compounds, Elsevier, N.Y. (1965).

U.S. Atomic Energy Commission, 1974a, "Generic Enviro l Statement--Mixed Oxide Fuel" (draft), Wash-1327, 4 vol. (1974,

U.S. Atomic Energy Commission, 1974b, "Reactor Safety Study: An Assessment of Accident Risks in U.S. Commercial Nuclear Power Plants," Wash-1400-D (1974).

U.S. Geological Survey, 1970, The National Atlas: the United States of America, Washington (1970).

Warren, C. E., Biology and Water Pollution Control, Saunders (1971).

Weast, R. C., ed., Handbook of Chemistry and Physics, 56th ed., Chemical Rubber Company, Cleveland, Ohio (1975).

Wilson, W. E., Jr., "A Critical Review of Gas-Phase Reaction Kinetics of Hydroxy (Radical)," *J. Chem. Phys. Ref. Data*, 1(2) 535 (1972).

Abstracting Services

Biological Abstracts, Biosciences Information Services (BA)

Chemical Abstracts, American Chemical Society (CA)

Index Medicus, Government Printing Office (IM)

Computer-Based Literature Search Services

CHEMLINE, National Library of Medicine (CHEMLINE)

Chemical Biological Activities, Literature of Interactions of Chemical Substances with Biological Systems, Chemical Abstracts System (CBAC)

Environmental Mutagen Information Center, Oak Ridge National Laboratory (EMIC)

Toxic Materials Information Center, Oak Ridge National Laboratory (TMIC)

TOXLINE, National Library of Medicine (TOXLINE)

Periodicals

Chemical Marketing Reporter, Schnell Publishing Co., New York (CMR)

Journal of the Water Pollution Control Federation, Water Pollution Control Federation, Washington (JWPCF)

Computer-Based Data Files

Commission of the European Communities, Economic Data on Carbamates, Organo-Chlorine Chemicals, and Organo-Phosphorus Chemicals, SRI (EEC)

National Cancer Institute, Chemicals That Impact on Man and His Environment (NCI)

National Emissions Data System, EPA-OAWM (NEDS)

Storage and Retrieval of Aerometric Data EPA-OAWM (SAROAD)

Storage and Retrieval of Water Data EPA-OWHM (STORET)

Technical Assistance Data System EPA-OHM (TADS)

Toxicology Data Bank NLM (TDB)